Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for

Chiral Self-Recognition in a Bispericyclic Cyclodimerisation Reaction of 1-Azadienes.

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I. General information

All reagents and solvents were purchased from commercial sources, duly preserved, treated in the manner specified by the manufacturer and used without purification unless otherwise mentioned. Secondary monitoring of the reactions was carried out by TLC, using silica gel plates (Alugram, SIL, G/UV254) developed using VL-6C UV lamps (λ = 254 nm). On some occasions, it was necessary to develop with $KMnO_4$, to get a better view of the majority of the stains. The products were purified by column chromatography over silica gel (200-400 size). ^{1}H, ^{13}C and ^{19}F Nuclear Magnetic Resonance (NMR) spectra were recorded at 25 °C on a Bruker Advance 400 (at 400 MHz, 101 MHz and 282 MHz respectively), and TMS was used as internal standard for ^{1}H and ^{13}C, and HF for ^{19}F nucleus. Infrared spectra were recorded using a Nicolet iS10 FTIR spectrophotometer (Thermo Scientific), using the Smart iTR accessory and reporting the value of the peaks in cm^{-1}. IR spectra were taken as pure solids or oils. High resolution mass spectra (HRMS) were recorded by using Electrospray ionization (ESI) through a LC-QTOF method. X-ray data were obtained using an Agilent Technologies Super-Nova (Cu) diffractometer. Elemental analysis was conducted using Euro EA Elemental Analyzer (CHNS) from EuroVector. The removal of solvents was carried out using rotary evaporators Buchi R-100 and R-210.

II. NMR study of the reaction

Gradient Temperature Analysis

In a NMR tube, 1-(4-bromophenyl)-3-((4-bromophenyl)amino)-4- ((dimethylamino)methyl)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one **2a** (27 mg, 0.05 mmol) was introduced. The NMR tube was then evacuated and refilled with N_2 (g) for three cycles. Then, acetic anhydride (25 µL) and CDCl3 (300 µL) were added. After vigorous manual stirring, ^{1}H NMR was conducted enabling the observation of the acetylated product **3a**. After that, Et_3N (15 µL) was added and another NMR spectrum was recorded at room temperature, followed by a temperature ramp-up regimen with NMR spectra acquired at 5-degree intervals. Throughout the initial temperature increments (ranging from RT to 50°C), no significant changes were observed in the spectra after 30 minutes at each temperature. Consequently, a temperature of 55°C was determined as the optimum temperature for the generation of azadiene **4a**.

Note: During the initial three NMR acquisitions, the presence of residual starting material **2a** was discerned, attributable to the small quantity of acetic anhydride employed. Unfortunately, efforts to employ a higher amount of acetic anhydride during the experiment did not allow us to obtain clear spectra due to the suboptimal NMR shimming, resulting in inconclusive NMR spectra.

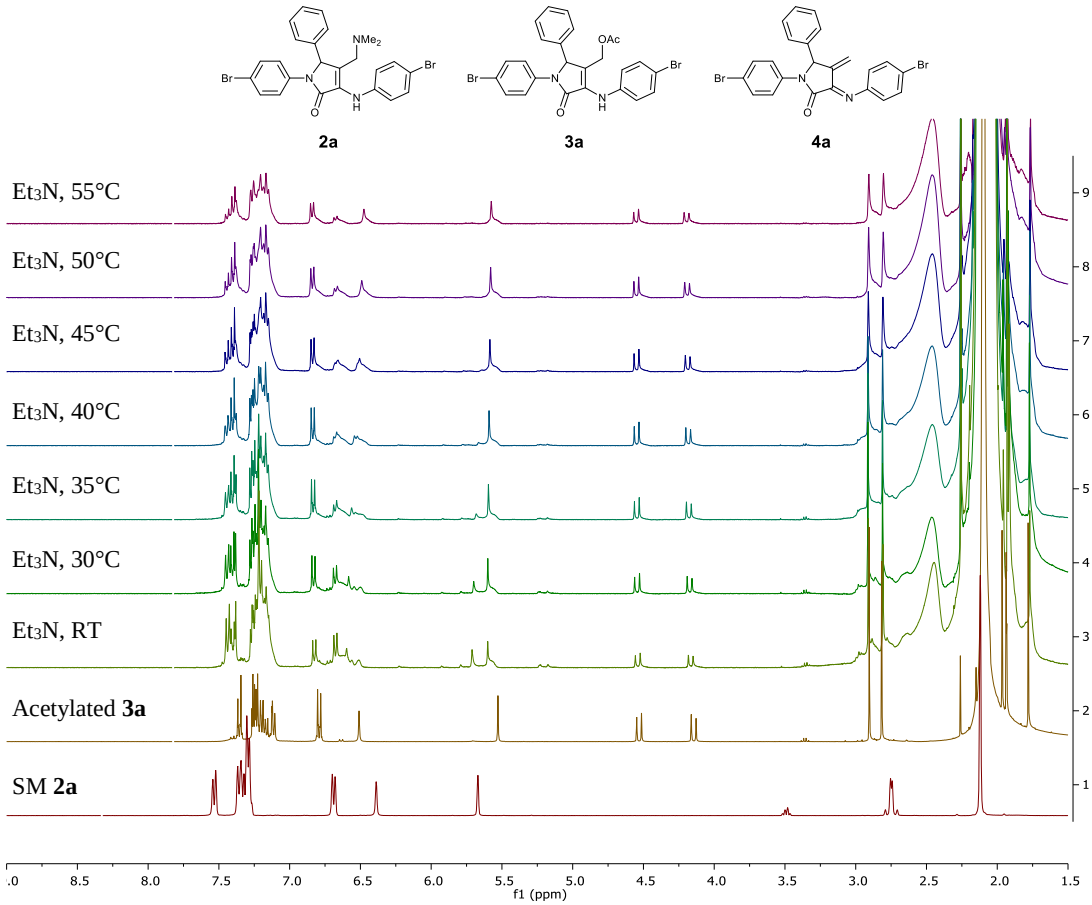
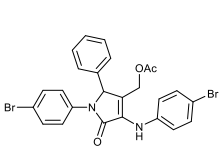


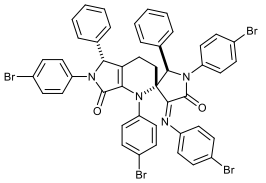
Figure S1. Temperature NMR study of the reaction.

Kinetic Study: 3a Disappearance vs 5a Formation

In a NMR tube, 1-(4-bromophenyl)-3-((4-bromophenyl)amino)-4-((dimethylamino)methyl)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one **2a** (27 mg, 0.05 mmol) was introduced. The NMR tube was then evacuated and refilled with N_2 (g) for three cycles. Then, acetic anhydride **3a** (25 µL) and $CDCl_3$ (300 µL) were added. After vigorous manual stirring, the generation of acetylated product **3a** was observed by ^1H NMR. Subsequently, Et_3N (15 µL) was added, and the temperature was raised to 55°C. Proton NMR measurements were taken every 30 minutes during 12 hours, and these data were employed to study the disappearance of the acetylated product **3a** and the formation of the dimer **5a** (Table S1. / Figure S2.).



3a



5a

Time / [h]	**3a** Disappearance / [%]	**5a** Formation / [%]
0	100	0
0.5	97	3
1	94	6
1.5	94	9
2	91	9
2.5	88	12
3	88	12
3.5	88	12
4	85	12
4.5	85	15
5	85	15
5.5	82	15
6	82	15
6.5	82	18
7	79	18
7.5	79	18
8	79	18
8.5	79	18
9	79	21
9.5	79	21
10	76	21
10.5	76	21
11	76	21
11.5	76	24
12	72	24

Table S1. 3a Disappearance vs **5a** Formation throughout12 reaction hours.

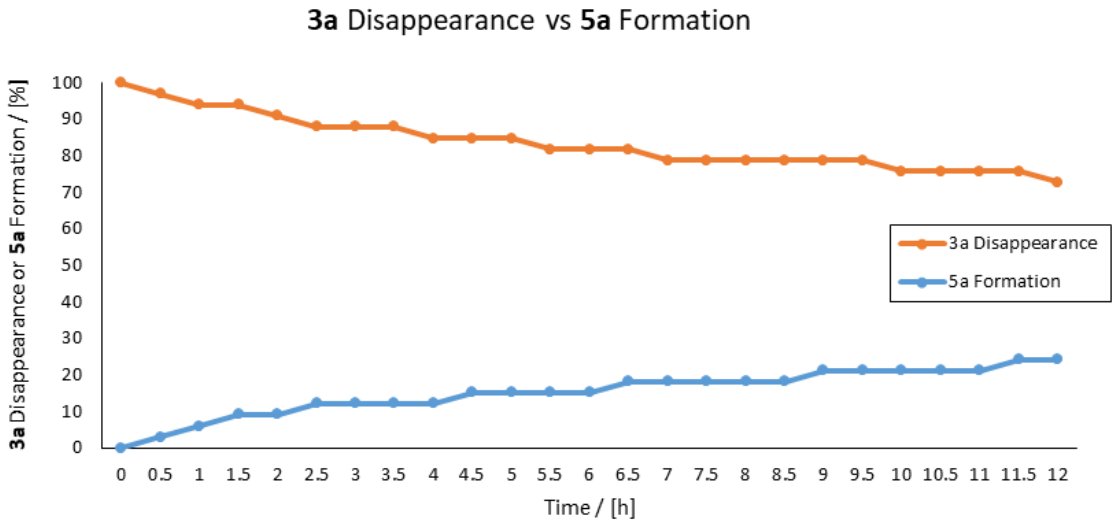
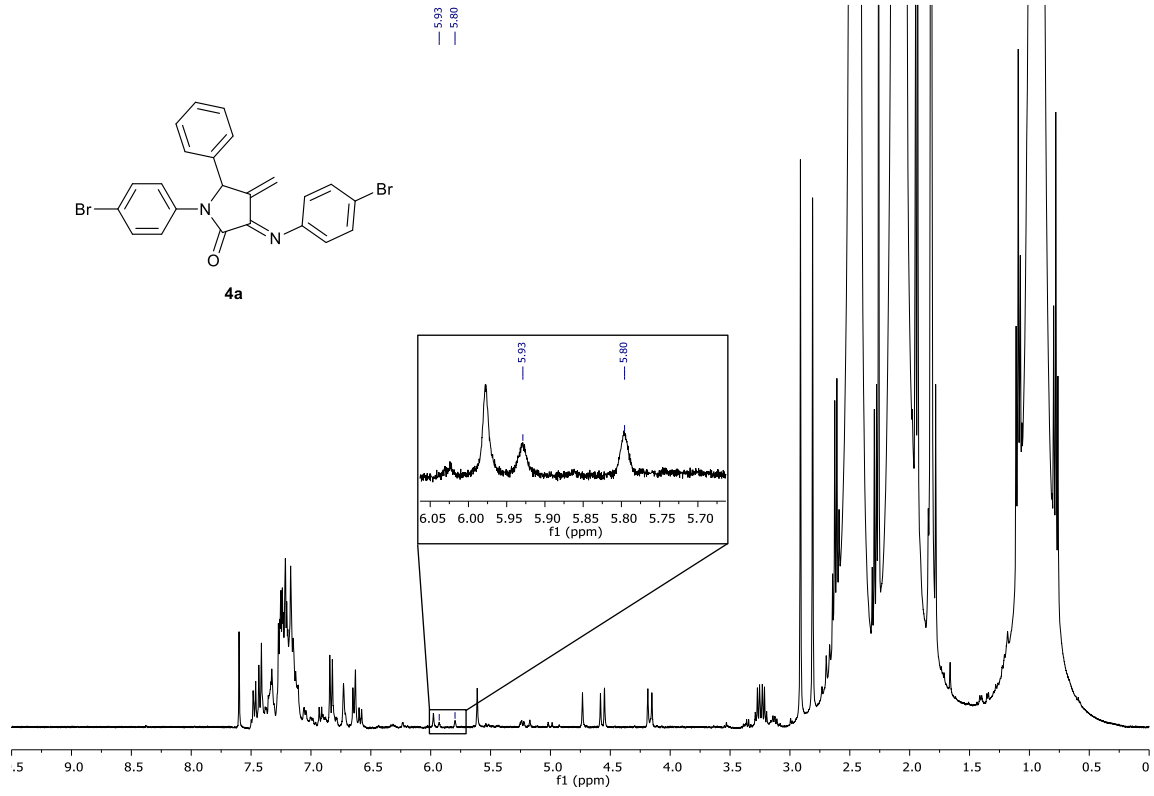


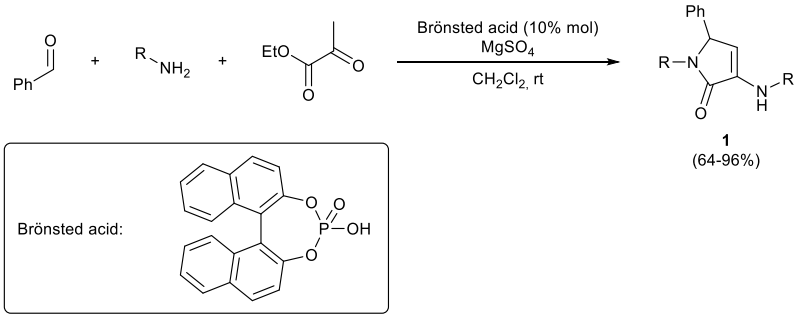
Figure S2. 3a Disappearance vs **5a** Formation throughout12 reaction hours.

Azadiene 4a Detection



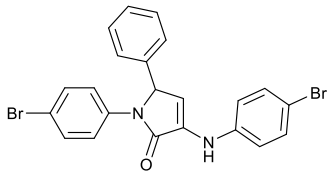
III. Synthesis and characterization data.

General procedure for the synthesis of γ-lactams 1



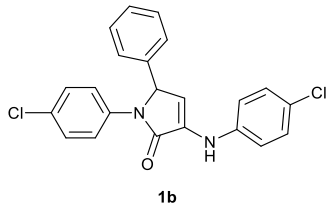
Following a literature procedure,[1] a solution of amine (2 equiv.), aldehyde (1 equiv.), ethyl pyruvate (3 equiv.) and binol-derived -phosphoric acid (10% mol) in CH_2Cl_2 (10 mL) was stirred overnight at room temperature in the presence of anhydrous $MgSO_4$. Next, the reaction was filtered and the resulting crude residue was purified by crystallization or flash column chromatography to afford pure 3-amino-3-pyrrolidin-2-ones **1**.

1-(4-Bromophenyl)-3-((4-bromophenyl)amino)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (1a). The general procedure was followed using *p*-bromoaniline (0.344 g, 2 mmol, 2 equiv.), benzaldehyde (0.102 mL, 1 mmol, 1 equiv.) and ethyl pyruvate (0.335 mL, 3 mmol, 3 equiv.), affording 0.396 g (82%) of **1a** as a white solid after column chromatography (Hexanes/AcOEt 8:2). **M.p.** (Et_2O): 225 – 226 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.45 (d, $^3J_{HH}$ = 9.0 Hz, 2H, 2×CH_{Ar}), 7.39 (d, $^3J_{HH}$ = 9.2 Hz, 2H, 2×CH_{Ar}), 7.38 (d, $^3J_{HH}$ = 8.9 Hz, 2H, 2×CH_{Ar}), 7.32–7.24 (m, 3H, 3×CH_{Ar}), 7.18 (d, $^3J_{HH}$ = 8.3 Hz, 2H, 2×CH_{Ar}), 6.94 (d, $^3J_{HH}$ = 8.9 Hz, 2H, 2×CH_{Ar}), 6.66 (s, 1H, NH), 6.05 (d, $^3J_{HH}$ = 2.6 Hz, 1H, =CH), 5.63 (d, $^3J_{HH}$ = 2.6 Hz, 1H, CHN) ppm. **^{13}C NMR {^{1}H}** (101 MHz, $CDCl_3$) δ 167.1 (C=O), 140.3 (C_{quat}), 136.9 (C_{quat}), 136.4 (C_{quat}), 132.4 (2×CH_{Ar}), 132.1 (2×CH_{Ar}), 131.8 (C_{quat}), 129.3 (2×CH_{Ar}), 128.6 (CH_{Ar}), 126.7 (2×CH_{Ar}), 122.9 (2×CH_{Ar}), 118.4 (2×CH_{Ar}), 118.1 (C_{quat}), 113.6 (C_{quat}), 108.9 (=CH), 64.3 (CHN) ppm. **FTIR** (neat) ν_{max}: 3327 (NH_{st}), 1672 ($C{=}O_{st}$), 1642 ($C{=}C_{st}$), 1073 ($C\text{-}Br_{st}$), 820 ($C\text{-}Br_{st}$) cm^{-1}. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_{22}H_{17}Br_2N_2O$ 482.9708, found 482.9715. Spectroscopic data are in agreement with the reported in the literature.[1c]


1a

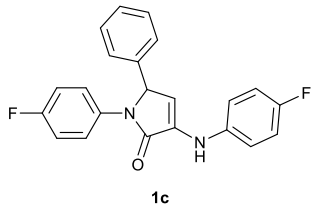
[1] (a) F. Palacios, J. Vicario and D. Aparicio. An Efficient Synthesis of Achiral and Chiral Cyclic Dehydro-α-Amino Acid Derivatives Through Nucleophilic Addition of Amines to β,γ-Unsaturated α-Keto Esters. *Eur. J. Org. Chem.*, 2006, 2843-2850. https://doi.org/10.1002/ejoc.200600092. (b) X. del Corte, A. Maestro, J. Vicario, E. Martínez de Marigorta, and F. Palacios. Brönsted-Acid-Catalyzed Asymmetric Three-Component Reaction of Amines, Aldehydes, and Pyruvate Derivatives. Enantioselective Synthesis of Highly Functionalized γ-Lactam Derivatives. *Org. Lett.*, 2018, **20**, 317-320. https://doi.org/10.1021/acs.orglett.7b03397. (c) X. del Corte, A. López-Francés, E. Martínez de Marigorta, F. Palacios and J. Vicario. Stereo- and Regioselective [3+3] Annulation Reaction Catalyzed by Ytterbium: Synthesis of Bicyclic 1,4-Dihydropyridines. *Adv. Synth. Catal.*, 2021, **363**, 4761-4769. https://doi.org/10.1002/adsc.202100785.

1-(4-Chlorophenyl)-3-((4-chlorophenyl)amino)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (1b). The general procedure was followed using *p*-chloroaniline (0.212 g, 2 mmol, 2 equiv.), benzaldehyde (0.102 mL, 1 mmol, 1 equiv.) and ethyl pyruvate (0.335 mL, 3 mmol, 3 equiv.), affording 0.304 g (77%) of **1b** as a white solid after crystallization (Et_2O). **M.p.** (Et_2O) = 207–209 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.53–7.46 (m, 2H, 2×CH_{Ar}), 7.33–7.26 (m, 3H, 3×CH_{Ar}), 7.26–7.22 (m, 4H, 4×CH_{Ar}), 7.19 (dd, $^3J_{HH}$ = 8.1, $^4J_{HH}$ = 1.6 Hz, 2H, 2×CH_{Ar}). 7.03–6.95 (m, 2H, 2×CH_{Ar}), 6.63 (s, 1H, NH), 6.05 (d, $^3J_{HH}$ = 2.6 Hz, 1H, =CH), 5.64 (d, $^3J_{HH}$ = 2.6 Hz, 1H, CHN) ppm. **^{13}C NMR {^{1}H}** (101 MHz, $CDCl_3$) δ 167.1 (C=O), 139.9 (C_{quat}), 137.0 (C_{quat}), 135.9 (C_{quat}), 131.9 (C_{quat}), 130.4 (C_{quat}), 129.5 (2×CH_{Ar}), 129.3 (2×CH_{Ar}), 129.2 (2×CH_{Ar}), 128.6 (CH_{Ar}), 126.8 (2×CH_{Ar}), 126.4 (C_{quat}), 122.6 (2×CH_{Ar}), 118.0 (2×CH_{Ar}), 108.7 (=CH), 64.3 (CHN) ppm. **FTIR** (neat) ν_{max}: 3328 (NH_{st}), 1664 ($C{=}O_{st}$), 1617 ($C{=}C_{st}$) cm^{-1}. **HRMS (ESI-TOF) m/z**: $[M+H]^+$ calcd for $C_{22}H_{17}Cl_2N_2O$ 395.0718, found 395.0715.



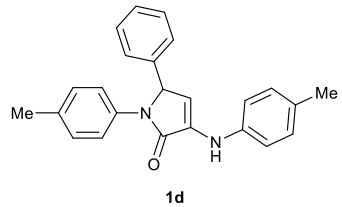
1b

1-(4-Fluorophenyl)-3-((4-fluorophenyl)amino)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (1c). The general procedure was followed, using *p*-fluoroaniline (0.222 g, 2 mmol, 2 equiv.), benzaldehyde (0.102 mL, 1 mmol, 1 equiv.) and ethyl pyruvate (0.335 mL, 3 mmol, 3 equiv.) to afford 0.344 g (95%) of **1c** as a yellow solid after crystallization (Et_2O). **M.p.** (Et_2O) = 213–215 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.49–7.43 (m, 2H, 2×CH_{Ar}), 7.32–7.26 (m, 2H, 2×CH_{Ar}), 7.25–7.22 (m, 1H, CH_{Ar}), 7.20–7.16 (m, 2H, 2×CH_{Ar}), 7.04–6.93 (m, 6H, 6×CH_{Ar}), 6.55 (s, 1H, NH), 6.00 (d, $^3J_{HH}$ = 2.6 Hz, 1H, =CH), 5.61 (d, $^3J_{HH}$ = 2.6 Hz, 1H, CHN) ppm. **^{13}C NMR {^{1}H}** (101 MHz, $CDCl_3$) δ 167.2 (C=O), 160.0 (d, $^1J_{FC}$ = 245.1 Hz, C_{quat}), 157.8 (d, $^1J_{FC}$ = 240.7 Hz, C_{quat}), 137.5 (d, $^4J_{FC}$ = 2.4 Hz, C_{quat}), 137.2 (C_{quat}), 133.5 (d, $^4J_{FC}$ = 3.0 Hz, C_{quat}), 132.6 (C_{quat}), 129.2 (2×CH_{Ar}), 128.5 (CH_{Ar}), 126.9 (2×CH_{Ar}), 123.7 (d, $^2J_{FC}$ = 8.0 Hz, 2×CH_{Ar}), 118.4 (d, $^3J_{FC}$ = 7.7 Hz, 2×CH_{Ar}), 116.2 (d, $^3J_{FC}$ = 28.0 Hz, 2×CH_{Ar}), 115.9 (d, $^2J_{FC}$ = 28.0 Hz, 2×CH_{Ar}), 107.4 (=CH), 77.4 (CH), 64.7 (CHN) ppm. **^{19}F NMR {^{1}H}** (282 MHz, $CDCl_3$) δ –116.9, –121.9 ppm. **FTIR** (neat) ν_{max}: 3328 (NH_{st}), 1664 ($C{=}O_{st}$), 1615 ($C{=}C_{st}$) cm^{-1}. **HRMS (ESI-TOF) m/z**: $[M+H]^+$ calcd for $C_{22}H_{17}F_2N_2O$ 363.1309, found 363.1307.



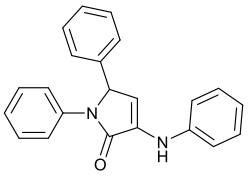
1c

5-Phenyl-1-(*p*-tolyl)-3-(*p*-tolylamino)-1,5-dihydro-2*H*-pyrrol-2-one (1d). The general procedure was followed using *p*-toluidine (0.215 g, 2 mmol, 2 equiv.), benzaldehyde (0.102 mL, 1 mmol, 1 equiv.) and ethyl pyruvate (0.335 mL, 3 mmol, 3 equiv.), affording 0.340 g (96%) of **1d** as a white solid after crystallization (Et_2O). **M.p.** (Et_2O): 214 - 215 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.40 (d, $^3J_{HH}$ = 8.5 Hz, 2H, 2×CH_{Ar}), 7.32 - 7.17 (m, 5H, 5×CH_{Ar}), 7.10 (d, $^3J_{HH}$ = 8.0 Hz, 2H, 2×CH_{Ar}), 7.09 (d, $^3J_{HH}$ = 8.0 Hz, 2H, 2×CH_{Ar}), 6.98 (d, $^3J_{HH}$ = 8.5 Hz, 2H, 2×CH_{Ar}), 6.58 (s, 1H, NH), 6.01 (d, $^3J_{HH}$ = 2.6 Hz, 1H, =CH), 5.63 (d, $^3J_{HH}$ = 2.6 Hz, 1H, CHN), 2.29 (s, 3H, CH_3), 2.26 (s, 3H, CH_3) ppm. **^{13}C NMR {^{1}H}** (101 MHz, $CDCl_3$) δ 167.0 (C=O), 138.8 (C_{quat}), 137.6 (C_{quat}), 134.8 (C_{quat}), 134.8 (C_{quat}), 132.0 (C_{quat}), 130.5 (C_{quat}), 129.9 (2×CH_{Ar}), 129.6 (2×CH_{Ar}), 129.0 (2×CH_{Ar}), 128.2 (CH_{Ar}), 126.9 (2×CH_{Ar}), 121.6 (2×CH_{Ar}), 116.8 (2×CH_{Ar}), 107.2 (=CH), 64.3 (CHN), 21.0 (CH_3), 20.8 (CH_3) ppm. **FTIR** (neat) ν_{max}: 3306 (NH_{st}), 1684 ($C{=}O_{st}$), 1665 ($C{=}C_{st}$) cm^{-1}. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_{24}H_{23}N_2O$ 355.1810, found 355.1805. Spectroscopic data are in agreement with the reported in the literature.[1b]



1d

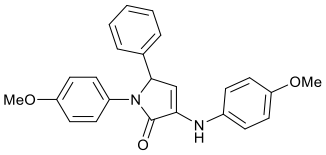
1,5-Diphenyl-3-(phenylamino)-1,5-dihydro-2*H*-pyrrol-2-one (1e). The general procedure was followed using aniline (0.182 mL, 2 mmol, 2 equiv.), benzaldehyde (0.102 mL, 1 mmol, 1 equiv.) and ethyl pyruvate (0.335 mL, 3 mmol, 3 equiv.), affording 0.212 g (65%) of **1e** as white crystals after crystallization (Et_2O).



1e

M.p. (Et_2O) = 224–225 °C. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 8.09 (s, 1H, NH), 7.62 (dd, $^3J_{HH}$ = 8.7 Hz, $^4J_{HH}$ = 1.2 Hz, 2H, 2×CH_{Ar}), 7.43–7.15 (m, 9H, 9×CH_{Ar}), 7.09–7.04 (m, 2H, 2×CH_{Ar}), 6.86 (tt, $^3J_{HH}$ = 7.0 Hz, $^4J_{HH}$ = 1.4 Hz, 2H, 2×CH_{Ar}), 6.34 (d, $^3J_{HH}$ = 2.7 Hz, 1H, =CH), 6.06 (d, $^3J_{HH}$ = 2.7 Hz, 1H, CHN) ppm. **^{13}C NMR {^{1}H}** (101 MHz, DMSO-d_6) δ 166.52 (C=O), 142.0 (C_{quat}), 138.0 (C_{quat}), 137.2 (C_{quat}), 131.8 (C_{quat}), 129.0 (2×CH_{Ar}), 128.8 (2×CH_{Ar}), 128.7 (2×CH_{Ar}), 127.7 (CH_{Ar}), 126.8 (2×CH_{Ar}), 124.4 (CH_{Ar}), 121.5 (2×CH_{Ar}), 120.2 (CH_{Ar}), 116.7 (2×CH_{Ar}), 109.8 (=CH), 62.4 (CHN) ppm. **FTIR** (neat) ν_{max}: 3303 (NH_{st}), 1681 ($C{=}O_{st}$), 1666 ($C{=}C_{st}$) cm^{-1}. **HRMS** (ESI-TOF) m/z: $[M+H]^+$, calcd for $C_{22}H_{19}N_2O$ 327.1497, found 327.1501.

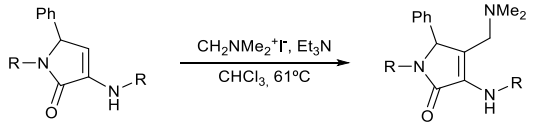
1-(4-Methoxyphenyl)-3-((4-methoxyphenyl)amino)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (1f). The general procedure was followed using *p*-anisidine (0.246 g, 2 mmol, 2 equiv.), benzaldehyde (0.102 mL, 1 mmol, 1 equiv.) and ethyl pyruvate (0.335 mL, 3 mmol, 3 equiv.), affording 0.300 g (78%) of **1f** as a white solid after column chromatography (Hexanes/AcOEt 8:2).



1f

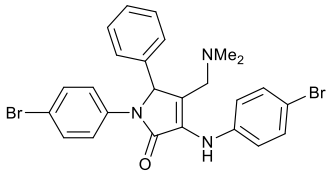
Mp (Et_2O): 198–200 °C. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.36 (d, $^3J_{HH}$ = 9.1 Hz, 2H, 2×CH_{Ar}), 7.30 - 7.16 (m, 5H, 5×CH_{Ar}), 7.03 (d, $^3J_{HH}$ = 8.9 Hz, 2H, 2×CH_{Ar}), 6.86 (d, $^3J_{HH}$ = 8.9 Hz, 2H, 2×CH_{Ar}), 6.81 (d, $^3J_{HH}$ = 9.1 Hz, 2H, 2×CH_{Ar}), 6.46 (bs, 1H, NH), 5.94 (d, $^3J_{HH}$ = 2.5 Hz, 1H, =CH), 5.57 (d, $^3J_{HH}$ = 2.5 Hz, 1H, CHN), 3.78 (s, 3H, CH_3), 3.74 (s, 3H, CH_3) ppm. **^{13}C NMR {^{1}H}** (75 MHz, $CDCl_3$) δ 167.3 (C=O), 157.1 (C_{quat}), 154.5 (C_{quat}), 137.8 (C_{quat}), 135.0 (C_{quat}), 133.1 (C_{quat}), 130.4 (C_{quat}), 129.0 (2×CH_{Ar}), 128.2 (2×CH_{Ar}), 127.1 (2×CH_{Ar}), 123.9 (2×CH_{Ar}), 118.6 (2×CH_{Ar}), 114.8 (2×CH_{Ar}), 114.3 (2×CH_{Ar}), 106.3 (=CH), 64.9 (CHN), 55.7 (CH_3), 55.5 (CH_3) ppm. **FTIR** (neat) ν_{max}: 3304 (NH_{st}), 3017 ($=CH_{st}$), 1669 ($C{=}O_{st}$), 1659 ($C{=}C_{st}$), 1250 ($C{-}O_{st}$), 1032 ($C{-}O_{st}$) cm^{-1}. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd. for $C_{24}H_{23}N_2O_3$ 387.1709, found 387.1702. Spectroscopic data are in agreement with the reported in the literature.[1b]

General Procedure for the functionalization of γ-lactams 1 with Eschenmoser salt



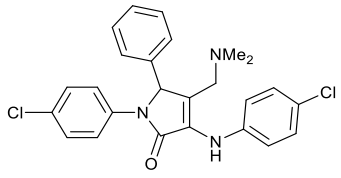
The corresponding 3-amino-3-pyrrolidin-2-one **1** (1 mmol, 1 equiv.) was stirred overnight with 1.5 equiv. of *N*,*N*-dimethylmethyleneiminium iodide (0.278 g, 1.5 mmol, 1.5 equiv.) in the presence of freshly distilled triethylamine (0.279 mL, 2.0 mmol, 2 equiv.) in refluxing chloroform (3 mL) under N_2 atmosphere. The reaction crude was acidified with 0.5 M HCl aqueous solution and extracted with dichloromethane (2 × 20 mL). The combined organic layers were dried with $MgSO_4$ and purified by column chromatography, affording the corresponding pure functionalized γ-lactams **2**. In some cases, other purification processes were necessary as detailed for each compound.

1-(4-Bromophenyl)-3-((4-bromophenyl)amino)-4-((dimethylamino)methyl)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (2a). The general procedure was followed using 1-(4-bromophenyl)-3-((4-bromophenyl)amino)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one **1a** (0.484 g, 1 mmol, 1 equiv.), affording 0.504 g (93%) of **2a** as orange crystals after chromatography (Hexanes/ AcOEt 7:3) followed by crystallization (Et_2O /Pentane 1:3). **M.p.** (Et_2O /Pentane) = 139–141 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.53 (d, $^3J_{HH}$ = 7.6 Hz, 2H, 2×CH_{Ar}), 7.37–7.25 (m, 9H, 9×CH_{Ar}), 6.68 (d, $^3J_{HH}$ = 7.6 Hz, 2H, 2×CH_{Ar}), 6.38 (s, 1H, NH), 5.66 (s, 1H, CH), 2.76 (d, $^2J_{HH}$ = 14.5 Hz, 1H, C$\underline{H}_A$$CH_B$), 2.72 (d, $^2J_{HH}$ = 14.5 Hz, 1H, CH_AC$\underline{H}_B$), 2.11 (s, 6H, 2×NCH_3) ppm. **^{13}C NMR {^{1}H}** (101 MHz, $CDCl_3$) δ 167.5 (C=O), 141.8 (C_{quat}), 136.8 (C_{quat}), 136.8 (C_{quat}), 132.0 (2×CH_{Ar}), 131.9 (2×CH_{Ar}), 130.7 (C_{quat}), 130.6 (C_{quat}), 129.2(2×CH_{Ar}), 128.5 (CH_{Ar}), 126.8 (2×CH_{Ar}), 122.0 (2×CH_{Ar}), 119.7 (2×CH_{Ar}), 117.3 (C_{quat}), 113.6 (C_{quat}), 64.4 (CH), 55.5 (CH_2), 45.5 (2×NCH_3) ppm. **FTIR** (neat) ν_{max}: 3321 (NH_{st}), 1689 (C=O_{st}), 1604 (C=C_{st}) cm^{-1}. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{25}H_{24}Br_2N_3O$ 542.0286, found 542.0269.



2a

1-(4-Chlorophenyl)-3-((4-chlorophenyl)amino)-4-((dimethylamino)methyl)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (2b). The general procedure was followed using 1-(*p*-chlorophenyl)-3-((*p*-chlorophenyl)amino)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (0.395 g, 1 mmol, 1 equiv.) **1b** to afford 0.281 g (62%) of **2b** as red solid after a chromatography column (Hexanes/ AcOEt 8:2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.54 (d, $^3J_{HH}$ = 9.1 Hz, 2H, 2×CH_{Ar}), 7.34–7.23 (m, 5H, 5×CH_{Ar}), 7.18 (d, $^3J_{HH}$ = 9.0 Hz, 2H, 2×CH_{Ar}), 7.14 (d, $^3J_{HH}$ = 8.9 Hz, 2H, 2×CH_{Ar}), 6.72 (d, $^3J_{HH}$ = 8.9 Hz, 2H, 2×CH_{Ar}), 6.25 (s, 1H, NH), 5.62 (s, 1H, CH), 2.73 (d, $^2J_{HH}$ = 12.5 Hz, 1H, C$\underline{H}_A$$CH_B$), 2.59 (d, $^2J_{HH}$ = 12.5 Hz, 1H, CH_AC$\underline{H}_B$), 2.08 (s, 6H, 2×NCH_3) ppm. **^{13}C NMR {^{1}H}** (101 MHz, $CDCl_3$) δ 167.5 (C=O), 141.3 (C_{quat}), 136.9 (C_{quat}), 136.4 (C_{quat}), 130.8 (C_{quat}), 130.2 (C_{quat}), 129.6 (C_{quat}), 129.2 (2×CH_{Ar}), 129.1 (2×CH_{Ar}), 129.0 (2×CH_{Ar}), 128.5 (CH_{Ar}), 126.9 (2×CH_{Ar}), 126.5 (C_{quat}), 121.7 (2×CH_{Ar}), 119.6 (2×CH_{Ar}), 64.6 (CH), 55.6 (CH_2), 45.5 (2×NCH_3) ppm. **FTIR** (neat) ν_{max}: 3399 (N-H_{st}), 1695 (C=O_{st}) cm^{-1}. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for



2b

$C_{25}H_{24}Cl_2N_3O$ 452.1218, found 452.1228.

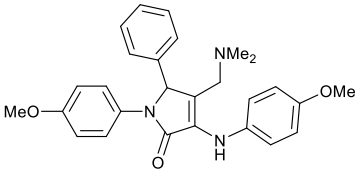
4-((Dimethylamino)methyl)-1-(4-fluorophenyl)-3-((4-fluorophenyl)amino)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (2c). The general procedure was followed using 1-(*p*-fluorophenyl)-3-((*p*-fluorophenyl)amino)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (0.362 g, 1 mmol, 1 equiv.) **1c** to afford 0.248 g (59%) of **2c** as white solid after a chromatography column (Hexanes/ AcOEt 8:2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56–7.48 (m, 2H, 2×CH_{Ar}), 7.33–7.20 (m, 5H, 5×CH_{Ar}), 6.98–6.86 (m, 4H, 4×CH_{Ar}), 6.82 (dd, $^3J_{HH}$ = 9.1 Hz, $^4J_{HH}$ = 4.7 Hz, 2H, 2×CH_{Ar}), 6.24 (s, 1H, NH), 5.61 (s, 1H, CH), 2.66 (m, 2H, CH_2), 2.06 (s, 6H, 2×NCH_3) ppm. **^{13}C NMR {^{1}H}** (101 MHz, $CDCl_3$) δ 167.6 (C=O), 159.5 (d, $^1J_{FC}$ = 244.2 Hz, C_{quat}), 158.4 (d, $^1J_{FC}$ = 240.5 Hz, C_{quat}), 138.5 (d, $^4J_{FC}$ = 2.6 Hz, C_{quat}), 137.1 (C_{quat}), 133.9 (d, $^4J_{FC}$ = 2.6 Hz, C_{quat}), 134.5 (C_{quat}), 129.1 (2×CH_{Ar}), 128.3 (CH_{Ar}) 127.3 (C_{quat}), 127.0 (2×CH_{Ar}), 122.6 (d, $^4J_{FC}$ = 8.1 Hz, 2×CH_{Ar}), 120.9 (d, $^3J_{FC}$ = 7.9 Hz, 2×CH_{Ar}), 115.8 (d, $^3J_{FC}$ = 1.3 Hz, 2×CH_{Ar}), 115.6 (d, $^3J_{FC}$ = 1.4 Hz, 2×CH_{Ar}), 64.9 (CH), 55.2 (CH_2), 45.5 (2×NCH_3) ppm. **^{19}F NMR {^{1}H}** (282 MHz, $CDCl_3$) δ –117.7, –121.5 ppm. **FTIR** (neat) ν_{max}: 3297 (N-H_{st}), 1699 (C=O_{st}) cm^{-1}. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{25}H_{24}F_2N_3O$ 420.1809, found 420.1819.

4-((Dimethylamino)methyl)-5-phenyl-1-(*p*-tolyl)-3-(*p*-tolylamino)-1,5-dihydro-2*H*-pyrrol-2-one (2d). The general procedure was followed, using 5-phenyl-1-(*p*-tolyl)-3-(*p*-tolylamino)-1,5-dihydro-2*H*-pyrrol-2-one **1d** (0.354 g, 1 mmol, 1 equiv.), affording 0.342 g (83%) of **2d** as red crystals after chromatography column (Hexanes/ AcOEt 8:2) followed by crystallization (Et_2O/Pentane 1:3). **M.p.** (Et_2O/Pentane) = 98–100 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.49 (d, $^3J_{HH}$ = 8.5 Hz, 2H, 2×CH_{Ar}), 7.33–7.29 (m, 4H, 4×CH_{Ar}), 7.25 (m, 1H, CH_{Ar}), 7.06 (d, $^3J_{HH}$ = 8.2 Hz, 2H, 2×CH_{Ar}), 7.02 (d, $^3J_{HH}$ = 8.2 Hz, 2H, 2×CH_{Ar}), 6.76 (d, $^3J_{HH}$ = 8.5 Hz, 2H, 2×CH_{Ar}), 6.12 (s, 1H, NH), 5.69 (s, 1H, CH), 2.78 (d, $^2J_{HH}$ = 13.9 Hz, 1H, C$\underline{H}_A$CH_B), 2.67 (d, $^2J_{HH}$ = 13.9 Hz, 1H, CH_AC$\underline{H}_B$), 2.28 (s, 3H, CH_{3Tol}), 2.24 (s, 3H, CH_{3Tol}), 2.11 (s, 6H, 2×NCH_3) ppm. **^{13}C NMR {^{1}H}** (101 MHz, $CDCl_3$) δ 167.7 (C=O), 140.1 (C_{quat}), 137.8 (C_{quat}), 135.4 (C_{quat}), 134.0 (C_{quat}), 131.3 (C_{quat}), 131.3 (C_{quat}), 129.6 (2×CH_{Ar}), 129.5 (2×CH_{Ar}), 128.9 (2×CH_{Ar}), 128.0 (2×CH_{Ar}), 127.2 (C_{quat}), 127.0 (2×CH_{Ar}), 120.1 (2×CH_{Ar}), 119.1 (CH_{Ar}), 64.6 (CH), 55.3 (CH_2), 45.5 (2×NCH_3), 20.9 (CH_{3Tol}), 20.8 (CH_{3Tol}) ppm. **FTIR** (neat) ν_{max}: 3331 (NH_{st}), 1689 (C=O_{st}), 1614 (C=C_{st}) cm^{-1}. **HRMS** (ESI-TOF) m/z: $[M - Me_2N]^+$, calcd for $C_{25}H_{23}N_2O$ 367.1810, found 367.1806.

4-((Dimethylamino)methyl)-1,5-diphenyl-3-(phenylamino)-1,5-dihydro-2*H*-pyrrol-2-one (2e). The general procedure was followed using 1,5-diphenyl-3-(phenylamino)-1,5-dihydro-2*H*-pyrrol-2-one (0.326 g, 1 mmol, 1 equiv.) **1e** to afford 0.314 g (82%) of **2e** as white crystals after a chromatography column (Hexanes/ AcOEt 8:2) followed by a crystallization (Et_2O/Pentane 1:3). **M.p.** (Et_2O/Pentane) = 140–142 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.56 (dd, $^3J_{HH}$ = 8.8 Hz, $^4J_{HH}$ =1.2 Hz, 2H, 2×CH_{Ar}), 7.28–7.32 (m, 4H, 4×CH_{Ar}), 7.21–7.16 (m, 3H, 3×CH_{Ar}), 7.15–7.11 (m, 2H, 2×CH_{Ar}), 6.99–6.94 (m, 1H, 1×CH_{Ar}), 6.84 (tt, $^3J_{HH}$ = 7.3 Hz, $^4J_{HH}$ =1.2 Hz, 1H, CH_{Ar}), 6.75 (dd, $^3J_{HH}$ = 8.8 Hz, $^4J_{HH}$ =1.2 Hz, 2H, 2×CH_{Ar}), 6.17 (s, 1H, NH), 5.67 (s, 1H, CH), 3.05–2.36 (m, 2H, CH_2), 2.04 (s, 6H, 2×NCH_3) ppm. **^{13}C NMR {^{1}H}** (101 MHz, $CDCl_3$) δ 167.8 (C=O),

142.8 (C_{quat}), 137.9 (C_{quat}), 137.5 (C_{quat}), 130.8 (C_{quat}), 129.4 (CH_{Ar}), 129.1 (2×CH_{Ar}), 129.0 (2×CH_{Ar}), 128.9 (2×CH_{Ar}), 128.1 (CH_{Ar}), 126.9 (2×CH_{Ar}), 124.4 (CH_{Ar}), 121.5 (CH_{Ar}), 120.6 (2×CH_{Ar}), 118.3 (2×CH_{Ar}), 64.5 (CH), 55.5 (CH_2), 45.5 (2×NCH_3) ppm. **FTIR** (neat) ν_{max}: 3039 (=CH_{st}), 1691 (C=O_{st}) cm^{-1}. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{25}H_{26}N_3O$ 384.2076, found 384.2074.

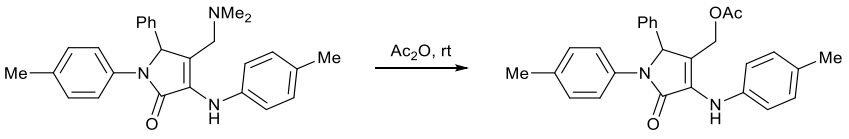
4-((Dimethylamino)methyl)-1-(4-methoxyphenyl)-3-((4-methoxyphenyl)amino)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (5f). The general procedure was followed using 1-(4-methoxyphenyl)-3-((4-methoxyphenyl)amino)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (0.386 g, 1 mmol, 1 equiv.) **1f** to afford 0.310 g (70%) of **2f** as an orange oil after a chromatography column (Hexanes/ AcOEt 8:2).



2f

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, $^3J_{HH}$ = 9.2 Hz, 2H, 2×CH_{Ar}), 7.31–7.27 (m, 5H, 5×CH_{Ar}), 6.89 (d, $^3J_{HH}$ = 8.9 Hz, 2H, 2×CH_{Ar}), 6.79 (d, $^3J_{HH}$ = 8.9 Hz, 2H, 2×CH_{Ar}), 6.78 (d, $^3J_{HH}$ = 9.2 Hz, 2H, 2×CH_{Ar}), 6.07 (s, 1H, NH), 5.63 (s, 1H, CH), 3.76 (s, 3H, OCH_3), 3.71 (s, 3H, OCH_3), 2.69 (d, $^2J_{HH}$ = 13.8 Hz, 1H, C$\underline{H}_A$CH_B), 2.61 (d, $^2J_{HH}$ = 13.8 Hz, 1H, CH_AC$\underline{H}_B$), 2.08 (s, 6H, 2×NCH_3) ppm. **^{13}C NMR {^{1}H}** (101 MHz, $CDCl_3$) δ 167.6 (C=O), 156.6 (C_{quat}), 155.6 (C_{quat}), 137.7 (C_{quat}), 135.4 (C_{quat}), 132.3 (C_{quat}), 131.5 (C_{quat}), 131.0 (C_{quat}), 128.9 (2×CH_{Ar}), 128.0 (2×CH_{Ar}), 127.2 (2×CH_{Ar}), 122.9 (2×CH_{Ar}), 122.4 (CH_{Ar}), 114.4 (2×CH_{Ar}), 114.2 (2×CH_{Ar}), 65.1 (CH), 55.6 (OCH_3), 55.4 (OCH_3), 54.7 (CH_2), 45.3 (2×NCH_3) ppm. **FTIR** (neat) ν_{max}: 3035 (=CH_{st}), 1688 (C=O_{st}) cm^{-1}. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{30}N_3O_3$ 444.2287, found 444.2277.

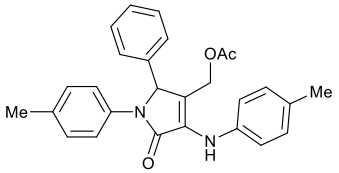
General Procedure for the synthesis of and isolation of acetylated lactam 3d



2d **3d**

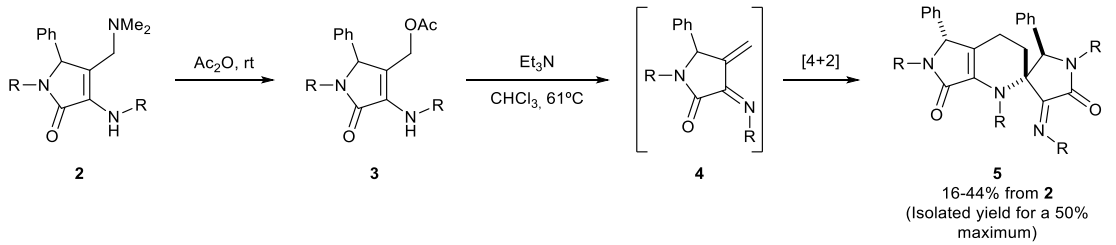
To a solution of 4-((dimethylamino)methyl)-5-phenyl-1-(*p*-tolyl)-3-(*p*-tolylamino)-1,5-dihydro-2*H*-pyrrol-2-one **2d** (0.367 g, 1 mmol, 1 equiv.) in chloroform (3 ml), 12 equivalents of acetic anhydride (1.1 ml) were added at room temperature. After 5 minutes, the solvent was evaporated and the obtained residue was dried in a vacuum pump, where the product crystallized spontaneously. The red crystals were washed with Et_2O, affording pure **3d**.

(5-Oxo-2-phenyl-1-(*p*-tolyl)-4-*(p*-tolylamino)-2,5-dihydro-1*H*-pyrrol-3-yl)methyl acetate (3d). The procedure was followed, affording 0.397 g (93%) of **3d** as red crystals. **M.p.** (Acetic acid) = 162–164 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 (d, $^3J_{HH}$ = 8.5 Hz, 2H, 2×CH_{Ar}), 7.32–7.19 (m, 5H, 5×CH_{Ar}), 7.07 (d, $^3J_{HH}$ = 8.3 Hz, 2H, 2×CH_{Ar}), 7.07 (d, $^3J_{HH}$ = 8.5 Hz, 2H, 2×CH_{Ar}), 6.96 (d, $^3J_{HH}$ = 8.3 Hz, 2H, 2×CH_{Ar}), 6.34 (s, 1H, NH), 5.57 (s, 1H, CH), 4.62 (d, $^2J_{HH}$ = 13.3 Hz, 1H, C$\underline{H}_A$CH_B), 4.22 (d, $^2J_{HH}$ = 13.3 Hz, 1H, CH_AC$\underline{H}_B$), 2.29 (s, 3H, CH_{3Tol}), 2.25 (s, 3H, CH_{3Tol}), 1.88 (s, 3H, CH_3).**^{13}C NMR {^{1}H}** (101 MHz, $CDCl_3$) δ 170.6 (C=O), 167.0 (C=O), 138.2 (C_{quat}), 136.7 (C_{quat}), 134.8 (C_{quat}), 134.6 (C_{quat}), 133.1 (C_{quat}), 132.6 (C_{quat}), 129.8 (2×CH_{Ar}), 129.6 (2×CH_{Ar}), 129.1 (2×CH_{Ar}), 128.5 (CH_{Ar}), 127.3 (2×CH_{Ar}), 121.9 (2×CH_{Ar}), 120.9 (2×CH_{Ar}), 115.3 (C_{quat}), 65.4 (CH), 58.1 (CH_2), 21.0 (CH_{3Tol}), 20.9 (CH_{3Tol}), 20.7 (CH_3) ppm. **FTIR** (neat) ν_{max}: 3388 (NH_{st}), 1739 (C=O_{st}), 1675 (C=O_{st}), 1615 (C=O_{st}) cm^{-1}. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{27}H_{27}N_2O_3$ 427.2022, found 427.2025.



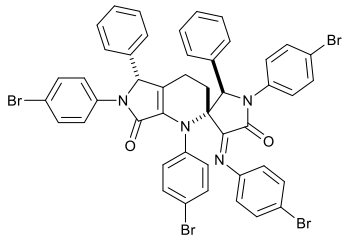
3d

General Procedure for the synthesis of spirocicles 5

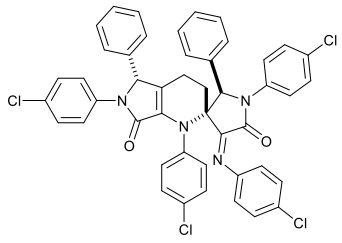


A solution of the corresponding functionalized γ-lactam **2** (1 mmol) in chloroform (3 ml) was stirred at room temperature under the presence of 12 equivalents of acetic anhydride. After 5 minutes the formation of the acetylated intermediate **3** was detected by NMR. Then, acetic acid was removed under low pressure and freshly distilled triethylamine (1.2 equiv.) and $CHCl_3$ were added to the reaction. The mixture was refluxed overnight. The reaction crude was acidified with 0.5 M HCl aqueous solution, and extracted with dichloromethane (2 × 20 mL). The combined organic layers were dried with $MgSO_4$ and purified by chromatography, affording the corresponding spirocyclic dihydropyridines **5**.

(2*R,3*R**,5'*R**,*Z*)-1,1',6'-Tris(4-bromophenyl)-4-((4-bromophenyl)imino)-2,5'-diphenyl-3',4',5',6'-tetrahydrospiro[pyrrolidine-3,2'-pyrrolo[3,4-*b*]pyridine]-5,7'(1'*H*)-dione (5a).** The general procedure was followed using 1-(4-bromophenyl)-3-((4-bromophenyl)amino)-4-((dimethylamino)methyl)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one **2a** (0.541 g, 1 mmol) to afford 0.377 g (38%) of **5a** as a brown oil after a chromatography column (Hexanes/ AcOEt 95:05). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.54–7.43 (m, 8H, 8×CH_{Ar}), 7.42–7.20 (m, 14H, 14×CH_{Ar}), 7.03 (d, $^3J_{HH}$ = 8.5 Hz, 2H, 2×CH_{Ar}), 6.26 (d, $^3J_{HH}$ = 8.4 Hz, 2H, 2×CH_{Ar}), 5.53 (s, 1H, CH), 4.89 (s, 1H, CH), 2.42–2.18 (m, 2H, 2×CH_2), 1.71 (m, 1H, CH_ACH_B), 1.46 (m, 1H, CH_ACH_B) ppm. **^{13}C NMR {^{1}H}** (101 MHz, $CDCl_3$) δ 166.0 (C_{quat}), 161.3 (C_{quat}), 157.3 (C_{quat}), 147.3 (C_{quat}), 142.0 (C_{quat}), 137.1 (C_{quat}), 137.0 (C_{quat}), 136.9 (C_{quat}), 135.5 (C_{quat}), 134.5 (C_{quat}), 133.5 (C_{quat}), 132.7 (2×CH_{Ar}), 132.2 (2×CH_{Ar}), 132.0 (2×CH_{Ar}), 131.9 (CH_{Ar}), 131.6 (2×CH_{Ar}), 129.9 (2×CH_{Ar}), 129.5 (CH_{Ar}), 129.5 (2×CH_{Ar}), 128.8 (2×CH_{Ar}), 126.0 (2×CH_{Ar}), 123.0 (2×CH_{Ar}), 122.1 (2×CH_{Ar}), 121.5 (2×CH_{Ar}), 121.4 (C_{quat}), 120.0 (C_{quat}), 119.4 (2×CH_{Ar}), 118.2 (C_{quat}), 117.2 (C_{quat}), 72.3 (CH), 66.9 (C_{quat}), 65.1 (CH), 24.6 (CH_2), 18.2 (CH_2) ppm. **FTIR** (neat) ν_{max}: 1699 (C=O_{st}), 1678 (C=N_{st}), 1607 (C=C_{st}) cm^{-1}. **HRMS** (ESI-TOF, APCI) product decomposition during analysis. Elem. Anal. % calcd. for $C_{46}H_{32}Br_4N_4O_2$ C, 55.67; H, 3.25; N, 5.65; found C, 55.55; H, 3.42; N, 5.66.

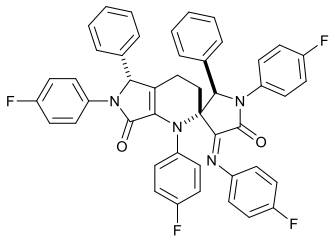

5a

(2*R,3*R**,5'*R**,Z)-1,1',6'-Tris(4-chlorophenyl)-4-((4-chlorophenyl)imino)-2,5'-diphenyl-3',4',5',6'-tetrahydrospiro[pyrrolidine-3,2'-pyrrolo[3,4-*b*]pyridine]-5,7'(1'H)-dione (5b).** The general procedure was followed using 1-(4-chlorophenyl)-3-((4-chlorophenyl)amino)-4-((dimethylamino) methyl)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one **2b** (0.452 g, 1 mmol) to afford 0.610 g (37%) of **5b** as yellow solid after a chromatography column (Hexanes/ AcOEt 9:1). **M.p.** (Et_2O) = 224–226 °C. **^{1}H NMR**


5b

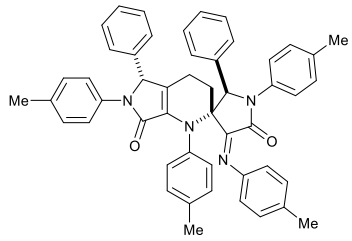
(400 MHz, $CDCl_3$) δ 7.62–7.40 (m, 6H, 6×CH_{Ar}), 7.40–6.96 (m, 18H, 18×CH_{Ar}), 6.35 (d, $^3J_{HH}$ = 8.6 Hz, 2H, 2×CH_{Ar}), 5.54 (s, 1H, CH), 4.91 (s, 1H, CH), 2.65–2.06 (m, 2H, 2×CH_2), 1.71 (m, 1H, $C\underline{H}_ACH_B$), 1.49 (m, 1H, $CH_AC\underline{H}_B$) ppm. **^{13}C NMR {^{1}H}** (101 MHz, $CDCl_3$) δ 166.0 (C_{quat}), 161.4 (C_{quat}), 157.4 (C_{quat}), 146.8 (C_{quat}), 141.5 (C_{quat}), 136.9 (C_{quat}), 136.5 (C_{quat}), 136.4 (C_{quat}), 135.5 (C_{quat}), 134.4 (C_{quat}), 133.6 (C_{quat}), 133.4 (C_{quat}), 132.1 (C_{quat}), 130.5 (C_{quat}), 129.8 (2×CH_{Ar}), 129.6 (2×CH_{Ar}), 129.5 (CH_{Ar}), 129.4 (C_{quat}), 129.2 (4×CH_{Ar}), 129.0 (4×CH_{Ar}), 128.8 (CH_{Ar}), 128.7 (4×CH_{Ar}), 126.0 (2×CH_{Ar}), 122.8 (2×CH_{Ar}), 121.3 (2×CH_{Ar}), 119.1 (2×CH_{Ar}), 72.4 (CH), 67.0 (C_{quat}), 65.2 (CH), 24.6 (CH_2), 18.2 (CH_2) ppm. **FTIR** (neat) ν_{max}: 1712 (C=O_{st}), 1682 (C=N_{st}), 1494 (C=C_{st}) cm^{-1}. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{46}H_{33}Cl_4N_4O_2$ 813.1358, found 813.1359.

(2*R,3*R**,5'*R**,*Z*)-1,1',6'-Tris(4-fluorophenyl)-4-((4-fluorophenyl)imino)-2,5'-diphenyl-3',4',5',6'-tetrahydrospiro[pyrrolidine-3,2'-pyrrolo[3,4-*b*]pyridine]-5,7'(1'*H*)-dione (5c).** The general procedure was followed using 4-((dimethylamino)methyl)-1-(4-fluorophenyl)-3-((4-fluorophenyl)amino)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one **2c** (0.419 g, 1 mmol) to afford 0.240 mg (16%) of **5c** as orange solid (Hexanes/ AcOEt 9:1). **M.p.** (Et_2O) = 192–194 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.60–7.39 (m, 6H, 6×CH_{Ar}), 7.35–7.22 (m, 7H, 7×CH_{Ar}), 7.24–7.14 (m, 2H, 2×CH_{Ar}), 7.06 (t, $^3J_{HH}$ = 8.3 Hz, 2H, 2×CH_{Ar}), 7.00–6.78 (m, 7H, 7×CH_{Ar}), 6.43 (dd, $^3J_{HH}$ = 8.8 Hz, $^4J_{FH}$ = 4.8 Hz, 2H, 2×CH_{Ar}), 5.53 (s, 1H, CH), 4.89 (s, 1H, CH), 2.40–2.21 (m, 2H, 2×CH_2), 1.73 (m, 1H, $C\underline{H}_ACH_B$), 1.52 (m, 1H, $CH_AC\underline{H}_B$) ppm. **^{13}C NMR {^{1}H}** (101 MHz, $CDCl_3$) δ 166.1 (C_{quat}), 161.7 (d, $^1J_{FC}$ = 247.5 Hz, C_{quat}), 160.8 (d, $^1J_{FC}$ = 247.5 Hz, C_{quat}), 160.4 (d, $^1J_{FC}$ = 243.7 Hz, C_{quat}), 161.5 (C_{quat}), 159.4 (d, $^1J_{FC}$ = 244.2 Hz, C_{quat}), 157.6 (C_{quat}), 144.2 (d, $^4J_{FC}$ = 2.9 Hz, C_{quat}), 139.0 (d, $^4J_{FC}$ = 3.1 Hz, C_{quat}), 137.0 (C_{quat}), 135.8 (C_{quat}), 134.0 (d, $^4J_{FC}$ = 3.0 Hz, C_{quat}), 133.9 (d, $^4J_{FC}$ = 2.8 Hz, C_{quat}), 133.9 (C_{quat}), 133.8 (C_{quat}), 129.7 (2×CH_{Ar}), 129.3 (2×CH_{Ar}), 128.7 (CH_{Ar}), 126.2 (2×CH_{Ar}), 123.9 (d, $^3J_{FC}$ = 8.3 Hz, 2×CH_{Ar}), 122.2 (d, $^3J_{FC}$ = 8.0 Hz, 2×CH_{Ar}), 119.7 (d, $^3J_{FC}$ = 8.1 Hz, 2×CH_{Ar}), 116.3 (CH_{Ar}), 116.1 (2×CH_{Ar}), 115.9 (2×CH_{Ar}), 115.8 (2×CH_{Ar}), 115.6 (2×CH_{Ar}), 115.4 (2×CH_{Ar}), 115.2 (2×CH_{Ar}), 72.9 (CH), 67.2 (C_{quat}), 65.5 (CH), 24.4 (CH_2), 18.1 (CH_2) ppm. **^{19}F NMR {^{1}H}** (282 MHz, $CDCl_3$) δ –114.0, –114.4, –118.0, –118.5 ppm. **FTIR** (neat) ν_{max}: 1708 (C=O_{st}), 1681 (C=N_{st}), 1503 (C=C_{st}) cm^{-1}. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{46}H_{32}F_4N_4O_2$ 749.2540, found 749.2526.



5c

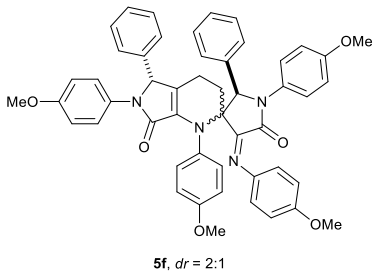
(2*R,3*R**,5'*R**,*Z*)-2,5'-Diphenyl-1,1',6'-tri-*p*-tolyl-4-(*p*-tolylimino)-3',4',5',6'-tetrahydrospiro[pyrrolidine-3,2'-pyrrolo[3,4-*b*]pyridine]-5,7'(1'*H*)-dione (5d).** The general procedure was applied starting from (5-oxo-2-phenyl-1-(*p*-tolyl)-4-(*p*-tolylamino)-2,5-dihydro-1*H*-pyrrol-3-yl)methyl acetate **3d** (0.451 g, 1 mmol) to afford 0.322 g (44%) of **5d** as a yellow oil after chromatography (Hexanes/ AcOEt 9:1). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.68–6.80 (m, 24H, 24×CH_{Ar}), 6.30 (d, $^3J_{HH}$ = 8.2 Hz, 2H, 2×CH_{Ar}), 5.52 (s, 1H, CH), 4.94 (s, 1H, CH), 2.54–2.05 (m, 2H, CH_2), 2.35 (s, 3H, CH_{3Tol}), 2.28 (s, 3H, CH_{3Tol}), 2.24 (s, 3H, CH_{3Tol}), 2.20 (s, 3H, CH_{3Tol}), 1.67 (m, 1H, $C\underline{H}_ACH_B$), 1.47 (m, 1H, $CH_AC\underline{H}_B$) ppm. **^{13}C NMR {^{1}H}** (101 MHz, $CDCl_3$) δ 166.2 (C_{quat}), 161.2 (C_{quat}), 157.6 (C_{quat}), 146.2 (C_{quat}), 140.4 (C_{quat}), 137.8 (C_{quat}), 136.8 (C_{quat}), 136.5 (C_{quat}), 135.9 (C_{quat}), 135.7 (C_{quat}), 135.5 (C_{quat}), 134.0 (C_{quat}), 133.9 (C_{quat}), 133.4 (C_{quat}), 132.6 (C_{quat}), 129.9 (2×CH_{Ar}), 129.8 (2×CH_{Ar}), 129.5 (CH_{Ar}), 129.4 (2×CH_{Ar}), 129.3 (2×CH_{Ar}), 129.2 (2×CH_{Ar}), 129.1 (CH_{Ar}),



5d

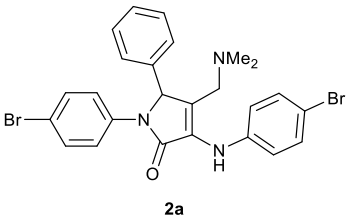
128.8 (2×CH_{Ar}), 128.7 (2×CH_{Ar}), 128.2 (2×CH_{Ar}), 126.1 (2×CH_{Ar}), 121.6 (2×CH_{Ar}), 120.1 (2×CH_{Ar}), 117.6 (2×CH_{Ar}), 72.3 (CH), 66.9 (C_{quat}), 65.0 (CH), 24.5 (CH_2), 21.1 (CH_3Tol), 21.0 (CH_3Tol), 20.9 (CH_3Tol), 20.7 (CH_3Tol), 18.1 (CH_2) ppm. **FTIR** (neat) ν_{max}: 1698 (C=O_{st}), 1669 (C=N_{st}), 1628 (C=C_{st}) cm^{-1}. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{50}H_{45}N_4O_2$ 733.3543, found 733.3537.

(2*R,5'*R**,*Z*)-1,1',6'-tris(4-methoxyphenyl)-4-((4-methoxyphenyl)imino)-2,5'-diphenyl-3',4',5',6'-tetrahydrospiro[pyrrolidine-3,2'-pyrrolo[3,4-*b*]pyridine]-5,7'(1'*H*)-dione (5f).** The general procedure was applied using 4-((dimethylamino)methyl)-1-(4-methoxyphenyl)-3-((4-methoxyphenyl)amino)-5-phenyl-1,5-dihydro-2H-pyrrol-2-one **2f** (0.444 g, 1 mmol) to afford 0.331 g (42%) of **5f** as a 2:1 mixture of the homodimer (2*R**,3*R**,5'*R**,*Z*) and heterodimer (2*R**,3*R**,5'*S**,*Z*) as an orange oil after chromatography (Hexanes/ AcOEt 9:1). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.55–7.13 (m, 24H, 24×CH_{Ar}), 6.93–6.66 (m, 12H, 12×CH_{Ar}), 6.61 (d, $^3J_{HH}$ = 8.7 Hz, 1H, 2×$CH_{Ar\ Minor}$), 6.53 (d, $^3J_{HH}$ = 8.7 Hz, 2H, 2×$CH_{Ar\ Major}$), 5.49 (s, 1H, CH_{Major}), 5.46 (s, 0.5H, CH_{Minor}), 5.21 (s, 0.5H, CH_{Minor}), 4.90 (s, 1H, CH_{Major}), 3.80 (s, 1.5H, $OCH_{3\ Minor}$), 3.78 (s, 3H, $OCH_{3\ Major}$), 3.78 (s, 1.5H, $OCH_{3\ Minor}$), 3.76 (s, 3H, $OCH_{3\ Major}$), 3.73 (s, 3H, $OCH_{3\ Major}$), 3.71 (s, 1.5H, $OCH_{3\ Minor}$), 3.69 (s, 3H, $OCH_{3\ Major}$), 3.69 (s, 1.5H, $OCH_{3\ Minor}$), 2.47–2.20 (m, 2H, $CH_{2\ Major}$), 2.12–1.89 (m, 2H, $CH_{2\ Major}$), 1.72–1.59 (m, 1H, $CH_{2\ Minor}$), 1.56–1.42 (m, 1H, $CH_{2\ Minor}$) ppm. **^{13}C NMR {^{1}H}** (101 MHz, $CDCl_3$) δ 166.2 ($C_{quat\ Major}$), 166.1 ($C_{quat\ Minor}$), 160.8 ($C_{quat\ Minor}$), 160.7 ($C_{quat\ Major}$), 158.6 ($C_{quat\ Minor}$), 158.5 ($C_{quat\ Major}$), 157.9 ($C_{quat\ Major}$), 157.8 ($C_{quat-\ Minor}$), 157.8 ($C_{quat\ Major}$), 157.7 ($C_{quat\ Minor}$), 157.3 ($C_{quat\ Minor}$), 157.3 ($C_{quat\ Major}$), 156.4 ($C_{quat\ Minor}$), 156.2 ($C_{quat\ Major}$), 141.4 ($C_{quat\ Major}$), 141.2 ($C_{quat\ Minor}$), 137.7 ($C_{quat\ Major}$), 137.2 ($C_{quat\ Minor}$), 136.8 ($C_{quat\ Minor}$), 136.6 ($C_{quat\ Major}$), 136.0 ($C_{quat\ Major}$), 134.9 ($C_{quat\ Minor}$), 134.2 ($C_{quat\ Major}$), 132.3 ($C_{quat\ Major}$), 131.4 ($C_{quat\ Major}$), 131.3 ($C_{quat\ Major}$), 131.1 ($C_{quat\ Minor}$), 131.1 ($C_{quat\ Minor}$), 129.8 ($C_{quat\ Minor}$), 129.5 (2×$CH_{Ar\ Major}$), 129.2 (2×$CH_{Ar\ Minor}$), 129.0 ($CH_{Ar\ Minor}$), 128.9 ($CH_{Ar\ Major}$), 128.4 ($CH_{Ar\ Minor}$), 128.3 ($CH_{Ar\ Major}$), 127.1 (2×$CH_{Ar\ Minor}$), 126.3 (2×$CH_{Ar\ Major}$), 123.8 (2×$CH_{Ar\ Minor}$), 123.7 (2×$CH_{Ar\ Major}$), 123.1 (2×$CH_{Ar\ Minor}$), 122.3 (2×$CH_{Ar\ Major}$), 120.8 (2×$CH_{Ar\ Minor}$), 120.3 (2×$CH_{Ar\ Major}$), 114.4 ($CH_{Ar\ Major}$ + $CH_{Ar\ Minor}$), 114.1 (2×$CH_{Ar\ Major}$), 114.0 (2×$CH_{Ar\ Minor}$), 114.0 (2×$CH_{Ar\ Major}$), 113.9 (2×$CH_{Ar\ Minor}$), 113.5 (2×$CH_{Ar\ Major}$), 113.5 (2×$CH_{Ar\ Minor}$), 72.9 (CH_{Major}), 71.6 (CH_{Minor}), 67.4 ($C_{quat\ Major}$), 67.0 ($C_{quat\ Minor}$), 65.6 (CH_{Major}), 65.4 (CH_{Minor}), 55.6 ($OCH_{3\ Major}$), 55.5 ($OCH_{3\ Minor}$), 55.5 (2×$OCH_{3\ Minor}$), 55.5 (2×$OCH_{3\ Major}$), 55.4 ($OCH_{3\ Major}$), 55.4 ($OCH_{3\ Minor}$), 24.8 ($CH_{2\ Minor}$), 24.6 ($CH_{2\ Major}$), 18.2 ($CH_{2\ Major}$), 17.7 ($CH_{2\ Minor}$) ppm. **FTIR** (neat) ν_{max}: 1692 (C=O_{st}), 1673 (C=N_{st}), 1606 (C=C_{st}) cm^{-1}. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{50}H_{45}N_4O_6$ 797.3339, found 797.3301.

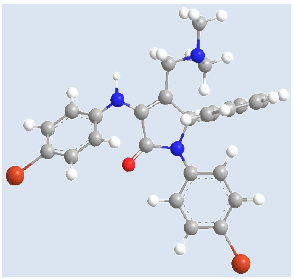


5f, *dr* = 2:1

IV. Crystallographic dato for 2a, 5a and 5b



2a



The structure of compound **2a** (b20220233_AL637DUCu2) was determined on a crystal prepared from a Et_2O/Pentane (1:3) solvent system by slow evaporation in a vial at room temperature. The X-ray data have been deposited at the Cambridge Crystallographic Data Centre (CCDC 2257284).

Intensity data were collected on an Agilent Technologies Super-Nova diffractometer, wich was equipped with monochromated Cu kα radiation (λ= 1.54184 Å) and de HyPix-6000H Hybrid Pixel Array Detecto. Measurement was carried out at 151.0 (6) K with the help of an Oxford Cryostream 700 PLUS temperature device. Data frames were processed (united cell determination, analytical absorption correction with face indexing, intensity data integration and correction for Lorentz and polarization effects) using the Crysalis software package.[2] The structure was solved using SHELXT[3] and refined by full-matrix least-squares with SHELXL-97.[4] Final geometrical calculations were carried out with Mercury[5] and PLATON[6] as integrated in WinGX[7] and Olex 2.

Experimental

Single crystals of **2a**. A suitable crystal was selected and monted on a SuperNova, Dual, Cu at home/near, HyPix diffractometer. The crystal was kept at 170.01(10) K during data collection. Using Olex2,[8] the structure was solved with the SHELXT[3] structure solution program using Intrinsic Phasing and refined with the SHELXL[4] refinement package using Least Squares minimisation.

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[2] CrysAlisPro, Agilent Technologies, Version 1.171.37.31 (release 14-01-2014 CrysAlis171 .NET) (compiled Jan 14 2014,18:38:05).

[3] G. M. Sheldrick. SHELXT - Integrated space-group and crystal-structure determination. *Acta Cryst.*, 2015, **A71**, 3-8. https://doi.org/10.1107/S2053273314026370.

[4] a). G. M. Sheldrick. A short history of SHELX. *Acta Cryst.*, 2008, **A64**, 112-122. https://doi.org/10.1107/S0108767307043930 b). G. M. Sheldrick. Crystal structure refinement with *SHELXL*. *Acta Cryst.*, 2015, **C71**, 3-8. https://doi.org/10.1107/S2053229614024218.

[5] C. F. Macrae. Mercury CSD 2.0 – new features for the visualization and investigation of crystal structures. *J. Appl. Crystallogr.*, 2008, **41**, 466-470. https://doi.org/10.1107/S0021889807067908.

[6] A. L. Spek. Single-crystal structure validation with the program *PLATON*. *J. Appl. Cryst.*, 2003, **36**, 7-13. https://doi.org/10.1107/S0021889802022112.

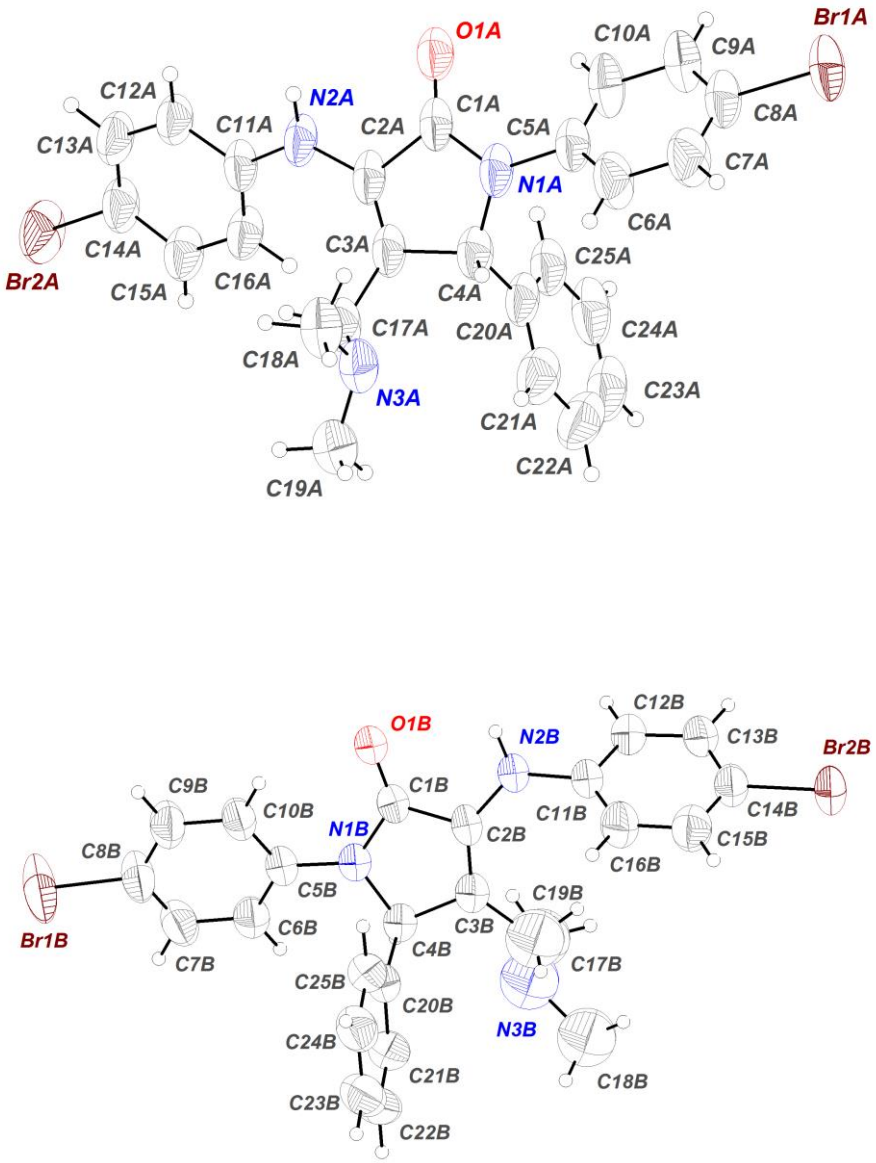
[7] L. J. Farrugia. *WinGX* suite for small-molecule single-crystal crystallography. *J. Appl. Cryst.*, 1999, **32**, 837-838. https://doi.org/10.1107/S0021889899006020.

[8] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann. OLEX2: A Complete Structure Solution, Refinement and Analysis Program. *J. Appl. Cryst.*, 2009, **42**, 339-341. https://doi.org/10.1107/S0021889808042726.

Crystal structure determination of 2a

Crystal Data for $C_{25}H_{23}Br_2N_3O$ (*M* =541.28 g/mol): triclinic, space group P-1 (no. 2), *a* = 13.2465(6) Å, *b* = 13.4713(5) Å, *c* = 15.1339(4) Å, *α* = 100.978(3)°, *β* = 98.736(3)°, *γ* = 115.947(4)°, *V* = 2297.76(15) Å3, *Z* = 4, *T* = 170.01(10) K, μ(CuKα) = 4.642 mm-1, *Dcalc* = 1.565 g/cm3, 45213 reflections measured (6.172° ≤ 2Θ ≤ 137.996°), 8531 unique (*R*int = 0.0634, Rsigma = 0.0408) which were used in all calculations. The final *R*1 was 0.0654 (I > 2σ(I)) and *wR*2 was 0.2027 (all data).

Thermal ellipsoid plot/ORTEP for compound 2a. Contour probability level: 50%



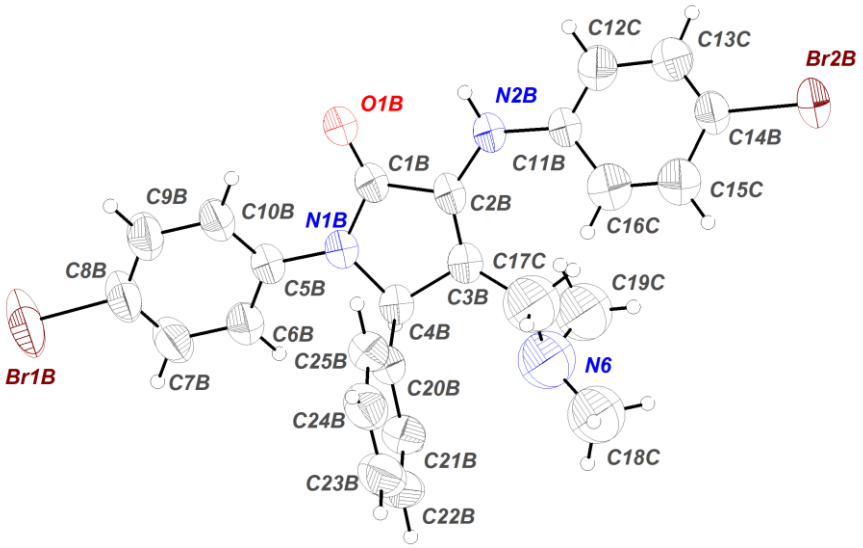
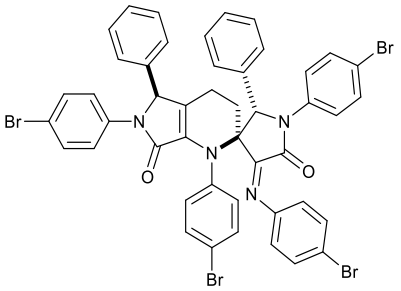


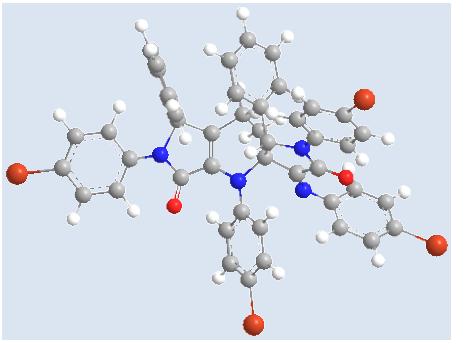
Table S2. Crystal data and structure refinement for 2a.

Identification code	b20220233_AL637DUCu2
Empirical formula	C25H23Br2N3O
Formula weight	541.28
Temperature/K	170.01(10)
Crystal system	triclinic
Space group	P-1
a/Å	13.2465(6)
b/Å	13.4713(5)
c/Å	15.1339(4)
α/°	100.978(3)
β/°	98.736(3)
γ/°	115.947(4)
Volume/Å^3	2297.76(15)
Z	4
ρcalcg/cm^3	1.565
μ/mm^{-1}	4.642
F(000)	1088.0
Crystal size/mm^3	0.26 × 0.13 × 0.108
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.172 to 137.996
Index ranges	-16 ≤ h ≤ 14, -16 ≤ k ≤ 16, -18 ≤ l ≤ 18
Reflections collected	45213
Independent reflections	8531 [Rint = 0.0634, Rsigma = 0.0408]
Data/restraints/parameters	8531/118/610
Goodness-of-fit on F2	1.067

Final R indexes [I>=2σ (I)]	R1 = 0.0654, wR2 = 0.1828
Final R indexes [all data]	R1 = 0.0885, wR2 = 0.2027
Largest diff. peak/hole / e Å^{-3}	0.92/-0.76



5a



The structure of compound **5a** (b20210012_AL467DUCu_auto) was determined on a crystal prepared from a Et_2O/Pentane (1:3) solvent system by slow evaporation in a vial at room temperature. The X-ray data have been deposited at the Cambridge Crystallographic Data Centre (CCDC 2125934).

Intensity data were collected on an Agilent Technologies Super-Nova diffractometer, wich was equipped with monochromated Cu kα radiation (λ= 1.54184 Å) and de HyPix-6000H Hybrid Pixel Array Detecto. Measurement was carried out at 151.0 (6) K with the help of an Oxford Cryostream 700 PLUS temperature device. Data frames were processed (united cell determination, analytical absorption correction with face indexing, intensity data integration and correction for Lorentz and polarization effects) using the Crysalis software package.[2] The structure was solved using SHELXT[3] and refined by full-matrix least-squares with SHELXL-97.[4] Final geometrical calculations were carried out with Mercury[5] and PLATON[6] as integrated in WinGX[7] and Olex 2. The asymmetric unit has two crystallization water molecules. These molecules are highly disordered and it has been impossible to make a model that results in a better according factor than if a squeeze is done eliminating the unassigned electron density, for this reason this model has been chosen.

Experimental

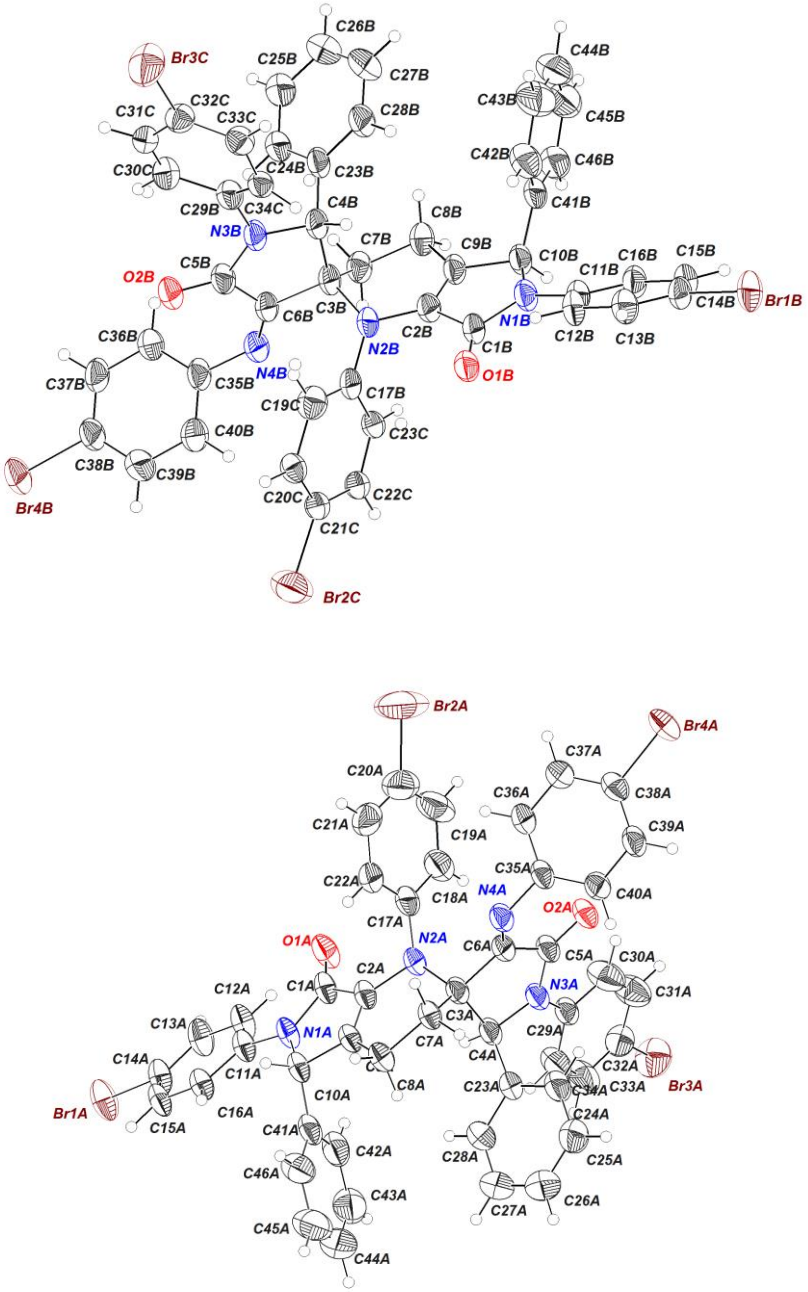
Single crystal of **5a**. A suitable crystal was selected and mounted on a SuperNova, Dual, Cu at home/near, HyPix diffractometer. The crystal was kept at 151.0(6) K during data collection. Using Olex2,[8] the structure was solved with the SHELXT[3] structure solution program using Intrinsic Phasing and refined with the SHELXL[4] refinement package using Least Squares minimisation.

Crystal structure determination of 5a.

Crystal Data for $C_{46}H_{32}Br_4N_4O_2$ (*M* =992.39 g/mol): triclinic, space group P-1 (no. 2), *a* = 13.0370(2) Å, *b* = 14.7579(2) Å, *c* = 23.6102(3) Å, *α* = 99.1840(10)°, *β* = 102.460(2)°, *γ* = 99.4360(10)°, *V* = 4284.98(11) Å3, *Z* = 4, *T* = 151.4(6) K, μ(CuKα) = 4.915 mm-1, *Dcalc* = 1.538 g/cm3, 85326 reflections measured (6.2° ≤ 2Θ ≤ 137.988°), 15665 unique (*R*int = 0.0750, Rsigma

= 0.0464) which were used in all calculations. The final *R*1 was 0.0520 (I > 2σ(I)) and *wR*2 was 0.1577 (all data).

Thermal ellipsoid plot/ORTEP for compound 5a. Contour probability level: 50%



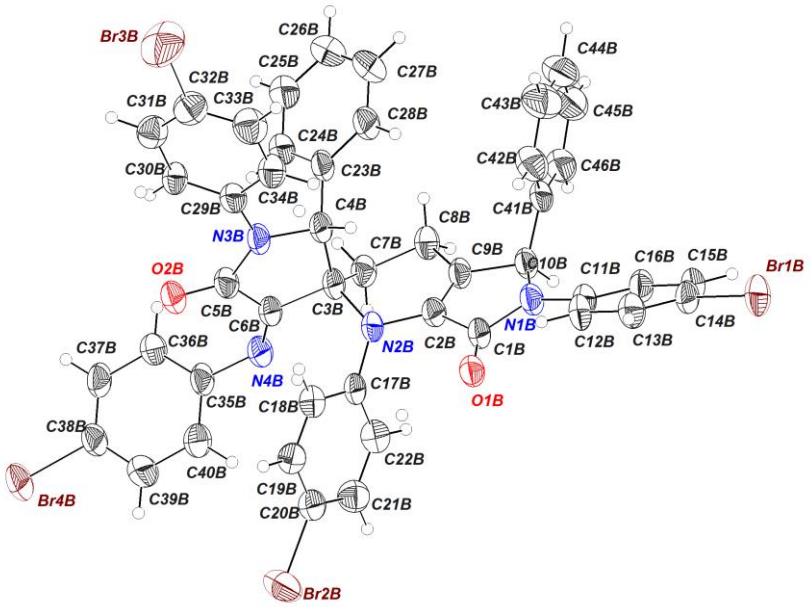
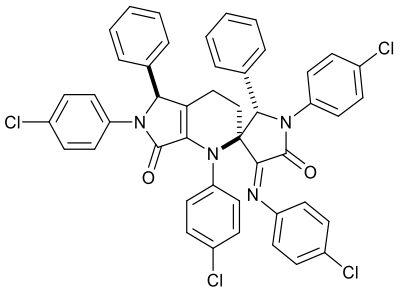


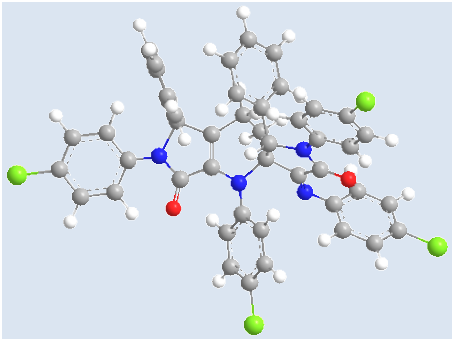
Table S3. Crystal data and structure refinement for 5a.

Identification code	b20210012_AL467DUCu_auto
Empirical formula	C46H32Br4N4O2
Formula weight	992.39
Temperature/K	151.4(6)
Crystal system	triclinic
Space group	P-1
a/Å	13.0370(2)
b/Å	14.7579(2)
c/Å	23.6102(3)
α/°	99.1840(10)
β/°	102.460(2)
γ/°	99.4360(10)
Volume/Å^3	4284.98(11)
Z	4
ρcalcg/cm^3	1.538
μ/mm^{-1}	4.915
F(000)	1968.0
Crystal size/mm^3	0.377 × 0.202 × 0.08
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.2 to 137.988
Index ranges	-14 ≤ h ≤ 15, -17 ≤ k ≤ 17, -28 ≤ l ≤ 28
Reflections collected	85326
Independent reflections	15665 [Rint = 0.0750, Rsigma = 0.0464]
Data/restraints/parameters	15665/144/1113
Goodness-of-fit on F2	1.081

Final R indexes [I>=2σ (I)]	R1 = 0.0520, wR2 = 0.1446
Final R indexes [all data]	R1 = 0.0679, wR2 = 0.1577
Largest diff. peak/hole / e Å^{-3}	1.54/-1.03



5b



The structure of compound **5b** (b20220253_AL649Et2ODDUCu) was determined on a crystal prepared from a $CDCl_3$ solvent system by slow evaporation in a vial at room temperature. The X-ray data have been deposited at the Cambridge Crystallographic Data Centre (CCDC 2257535).

Intensity data were collected on an Agilent Technologies Super-Nova diffractometer, wich was equipped with monochromated Cu kα radiation (λ= 1.54184 Å) and de HyPix-6000H Hybrid Pixel Array Detecto. Measurement was carried out at 151.0 (6) K with the help of an Oxford Cryostream 700 PLUS temperature device. Data frames were processed (united cell determination, analytical absorption correction with face indexing, intensity data integration and correction for Lorentz and polarization effects) using the Crysalis software package.[2] The structure was solved using SHELXT[3] and refined by full-matrix least-squares with SHELXL-97.[4] Final geometrical calculations were carried out with Mercury[5] and PLATON[6] as integrated in WinGX.[7] and Olex 2.

Experimental

Single crystal of **5b**. A suitable crystal was selected and mounted on a SuperNova, Dual, Cu at home/near, HyPix diffractometer. The crystal was kept at 151.0(6) K during data collection. Using Olex2,[8] the structure was solved with the SHELXT[3] structure solution program using Intrinsic Phasing and refined with the SHELXL[4] refinement package using Least Squares minimisation.

Crystal structure determination of 5b.

Crystal Data for $C_{46}H_{32}Cl_4N_4O_2$ (*M* =814.55 g/mol): monoclinic, space group P21/c (no. 14), *a* = 12.4973(4) Å, *b* = 13.4524(4) Å, *c* = 23.6777(8) Å, *β* = 101.817(3)°, *V* = 3896.3(2) Å3, *Z* = 4, *T* = 170.01(10) K, μ(CuKα) = 3.125 mm-1, *Dcalc* = 1.389 g/cm3, 49188 reflections measured (7.226° ≤ 2Θ ≤ 137.986°), 7243 unique (*R*int = 0.0969, Rsigma = 0.0745) which were used in all calculations. The final *R*1 was 0.0560 (I > 2σ(I)) and *wR*2 was 0.1747 (all data).

Thermal ellipsoid plot/ORTEP for compound 5b. Contour probability level: 50%

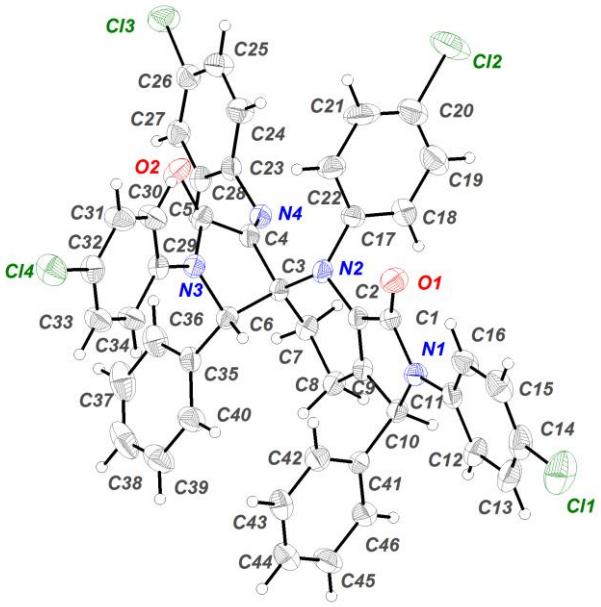


Table S4. Crystal data and structure refinement for 5b.

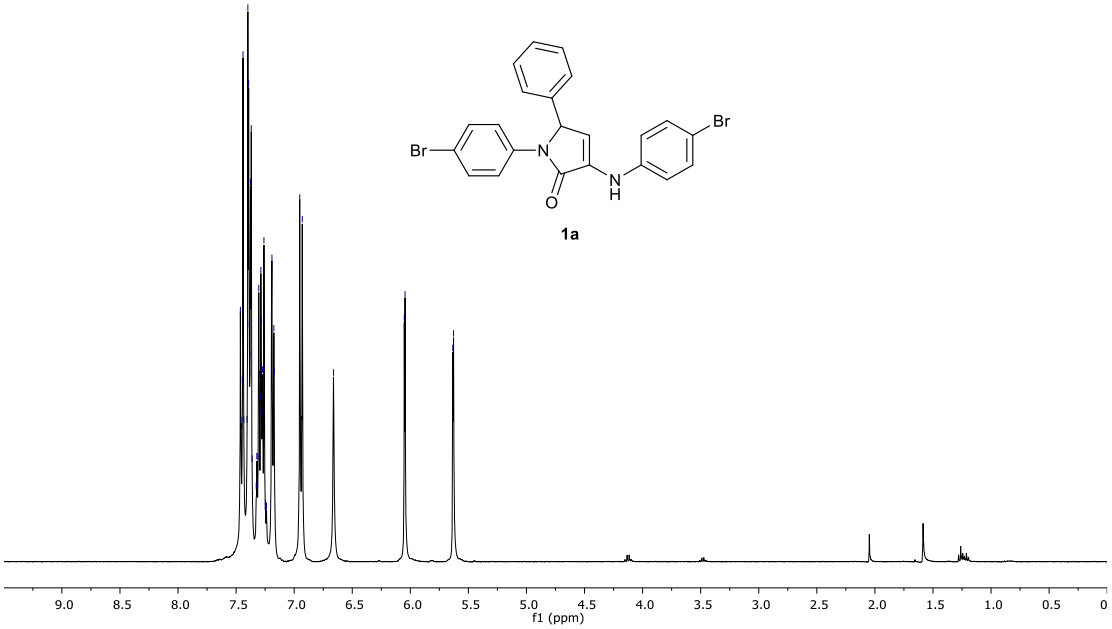
Identification code	b20220253_AL649Et2ODDUCu
Empirical formula	C46H32Cl4N4O2
Formula weight	814.55
Temperature/K	170.01(10)
Crystal system	monoclinic
Space group	P21/c
a/Å	12.4973(4)
b/Å	13.4524(4)
c/Å	23.6777(8)
α/°	90.0
β/°	101.817(3)
γ/°	90.0
Volume/Å^3	3896.3(2)
Z	4
ρcalcg/cm^3	1.389
μ/mm^{-1}	3.125
F(000)	1680.0
Crystal size/mm^3	0.140 × 0.103 × 0.053
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.226 to 137.986
Index ranges	-14 ≤ h ≤ 15, -16 ≤ k ≤ 16, -28 ≤ l ≤ 28
Reflections collected	49188
Independent reflections	7243 [Rint = 0.0969, Rsigma = 0.0745]

Data/restraints/parameters	7243/0/505
Goodness-of-fit on F2	1.050
Final R indexes [I>=2σ (I)]	R1 = 0.0560, wR2 = 0.1525
Final R indexes [all data]	R1 = 0.0840, wR2 = 0.1747
Largest diff. peak/hole / e $Å^{-3}$	0.83/-0.99

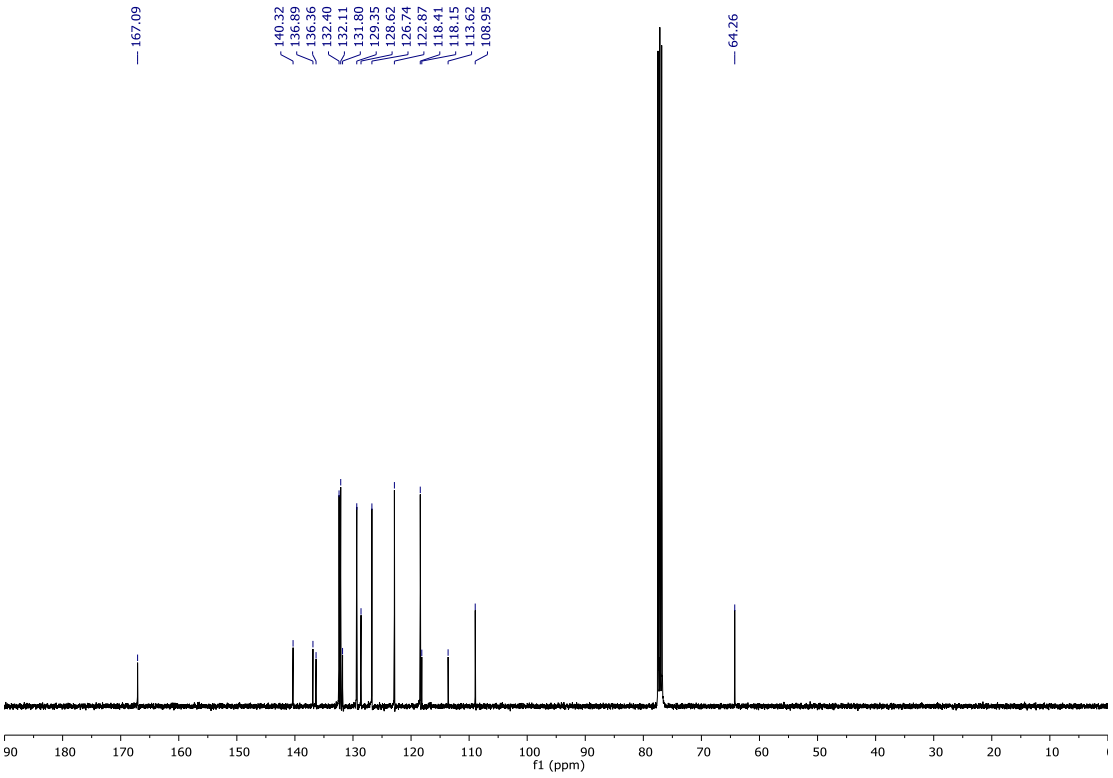
V. Copies of NMR spectra

1-(4-Bromophenyl)-3-((4-bromophenyl)amino)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (1a)

^{1}H NMR (400 MHz, $CDCl_3$)

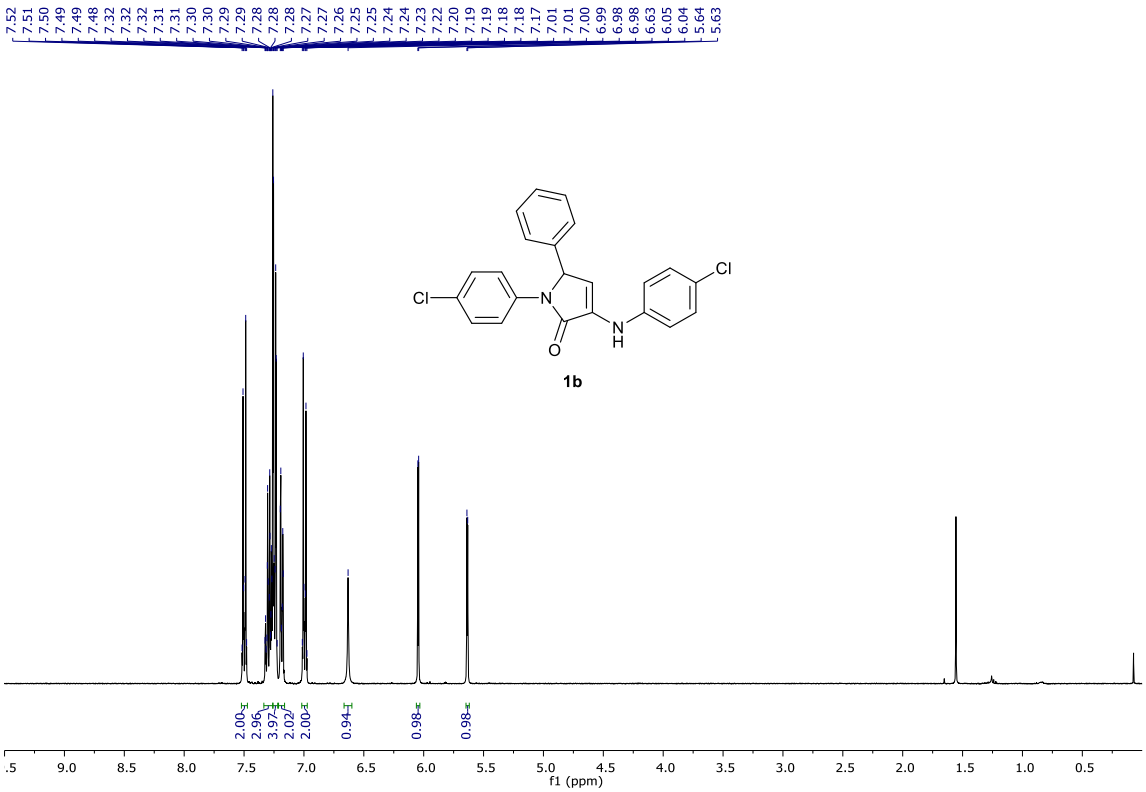


^{13}C NMR {^{1}H} (101 MHz, $CDCl_3$)

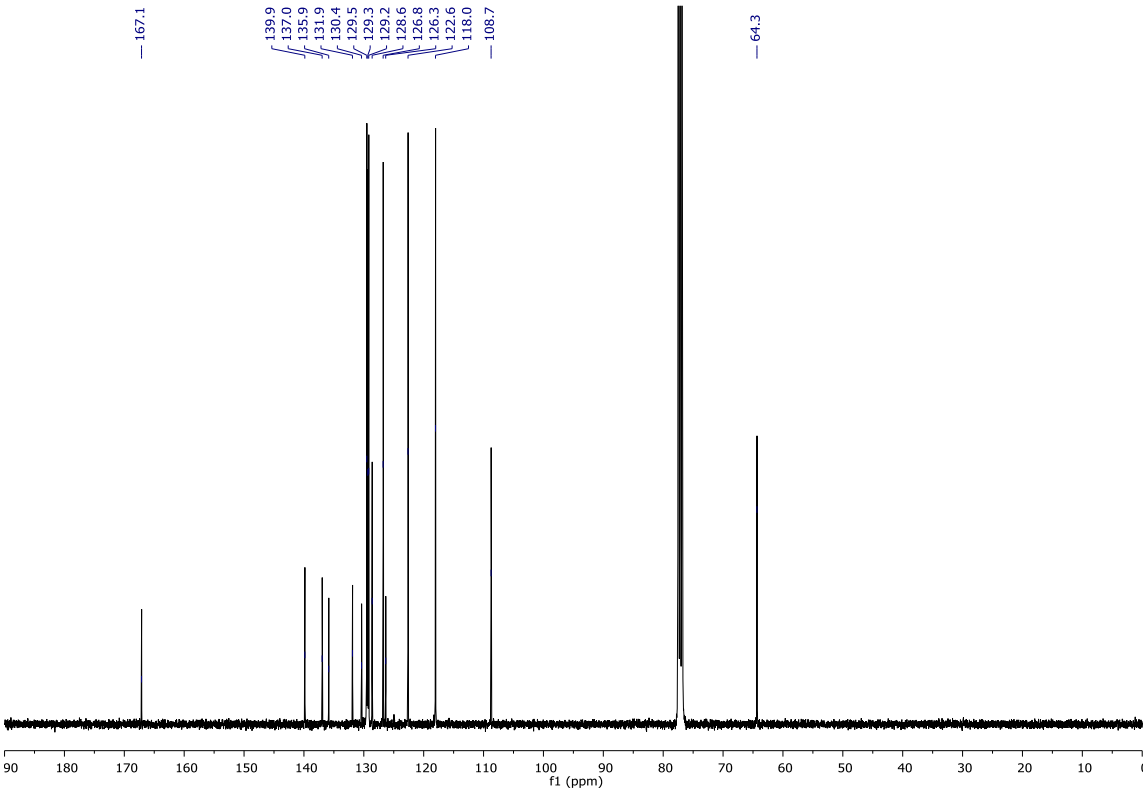


1-(4-Chlorophenyl)-3-((4-chlorophenyl)amino)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (1b)

^{1}H NMR (400 MHz, $CDCl_3$)

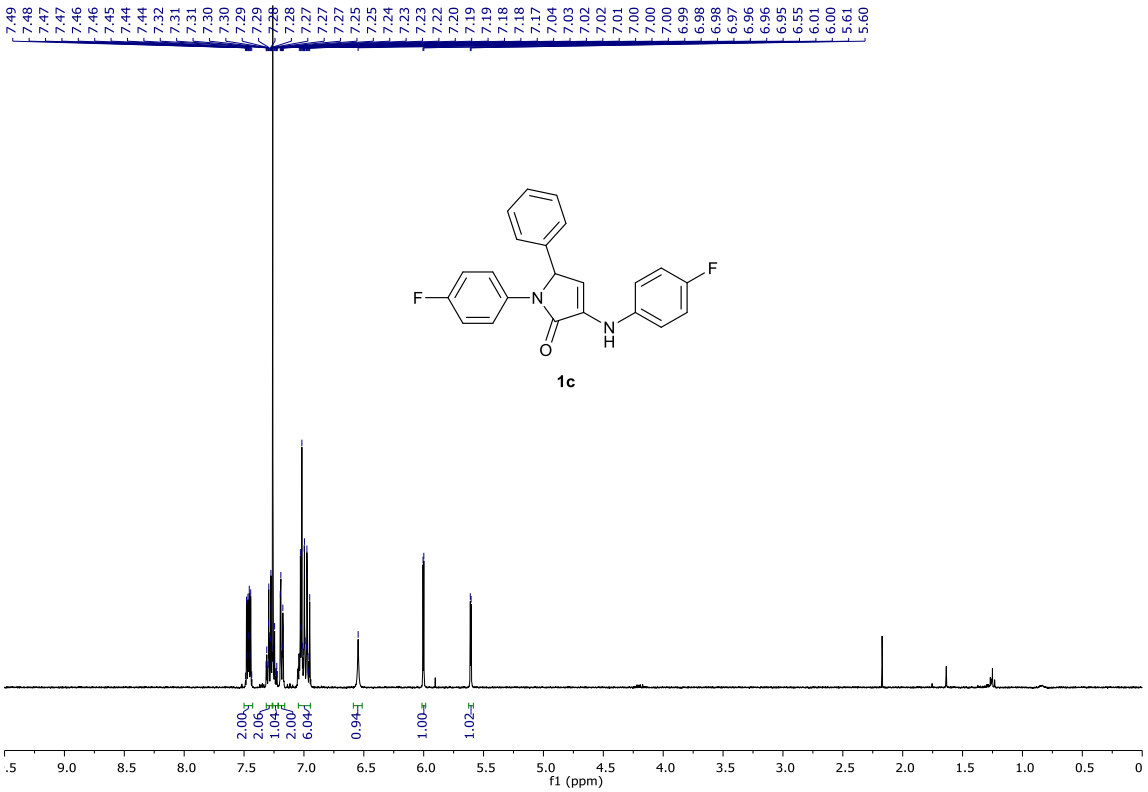


^{13}C NMR {^{1}H} (101 MHz, $CDCl_3$)

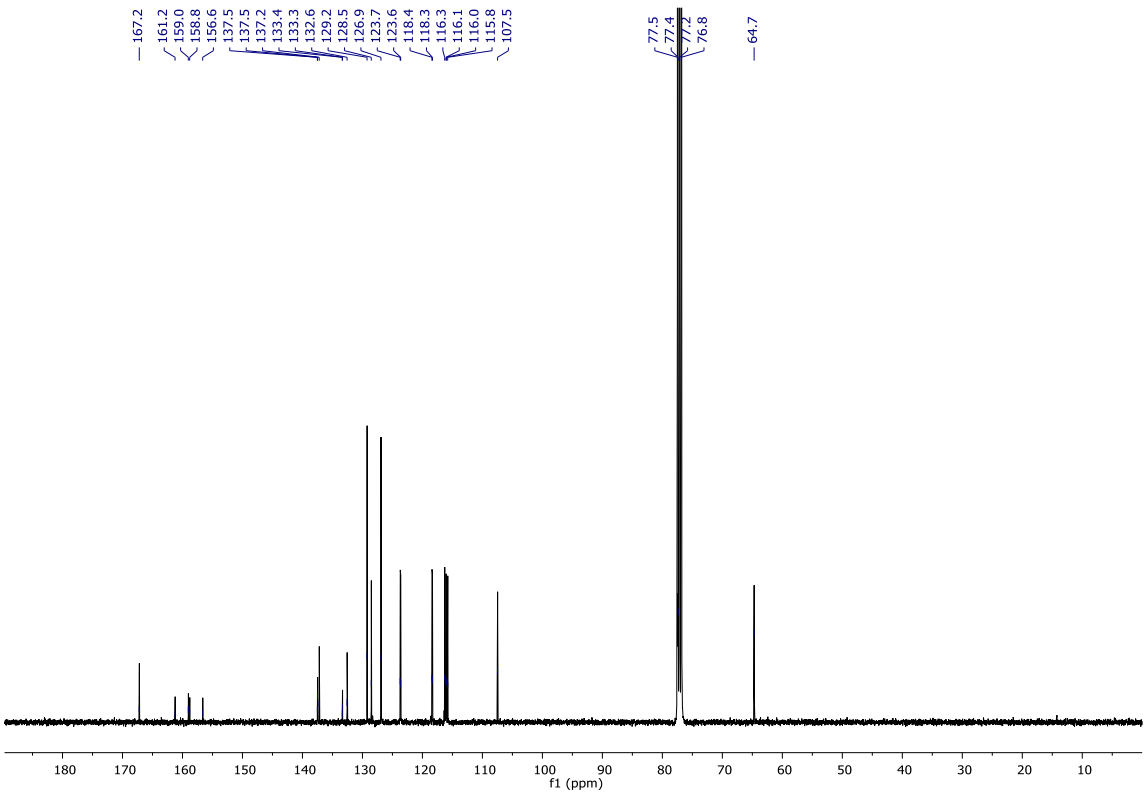


1-(4-Fluorophenyl)-3-((4-fluorophenyl)amino)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (1c)

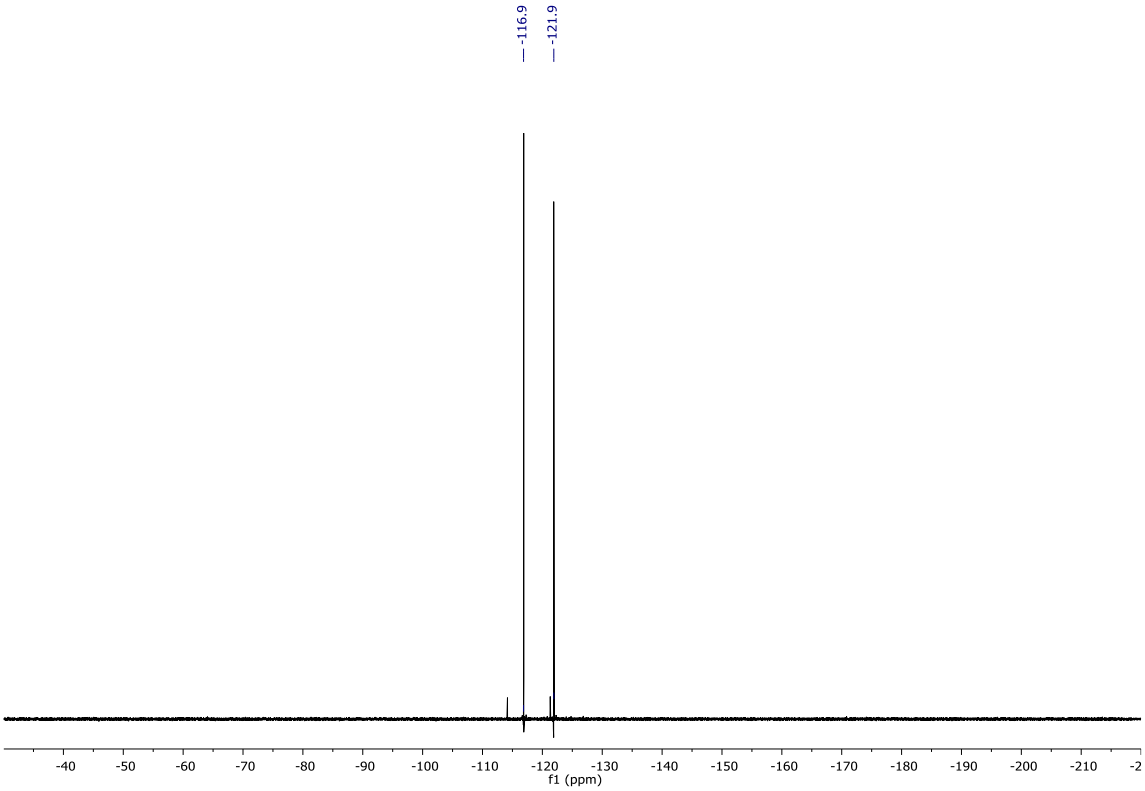
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR {^{1}H} (101 MHz, $CDCl_3$)

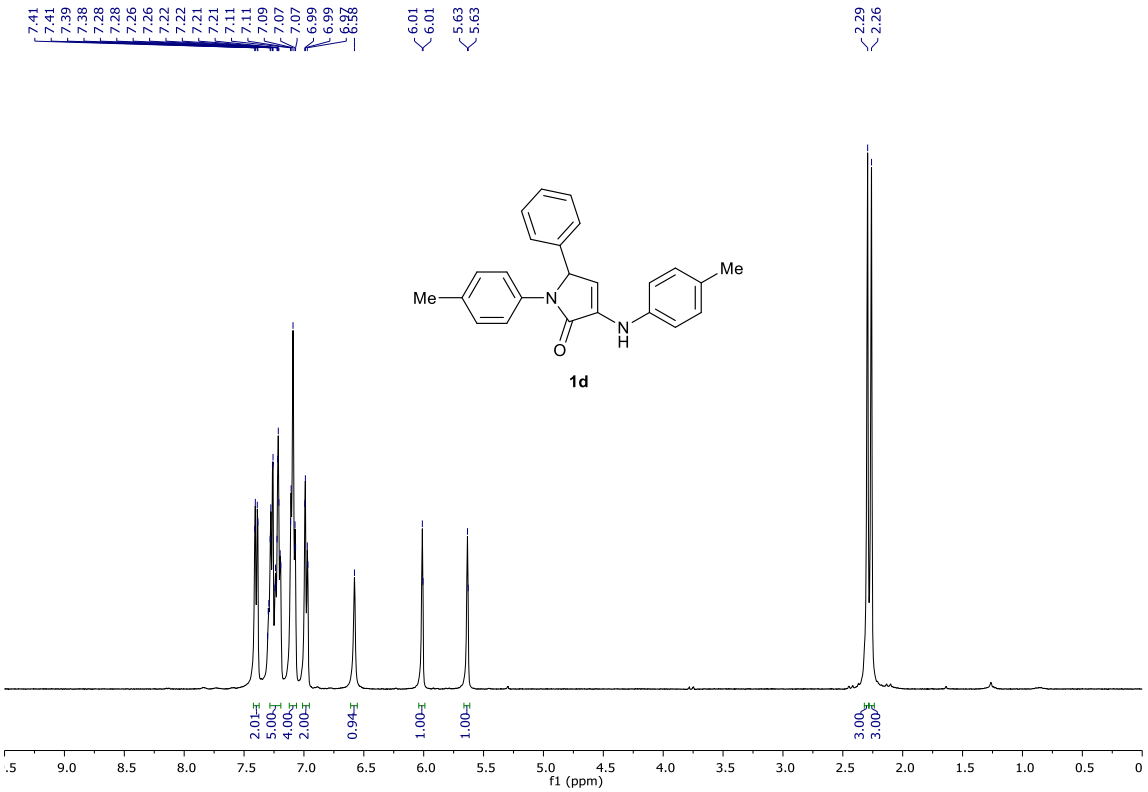


^{19}F NMR {^{1}H} (282 MHz, $CDCl_3$)

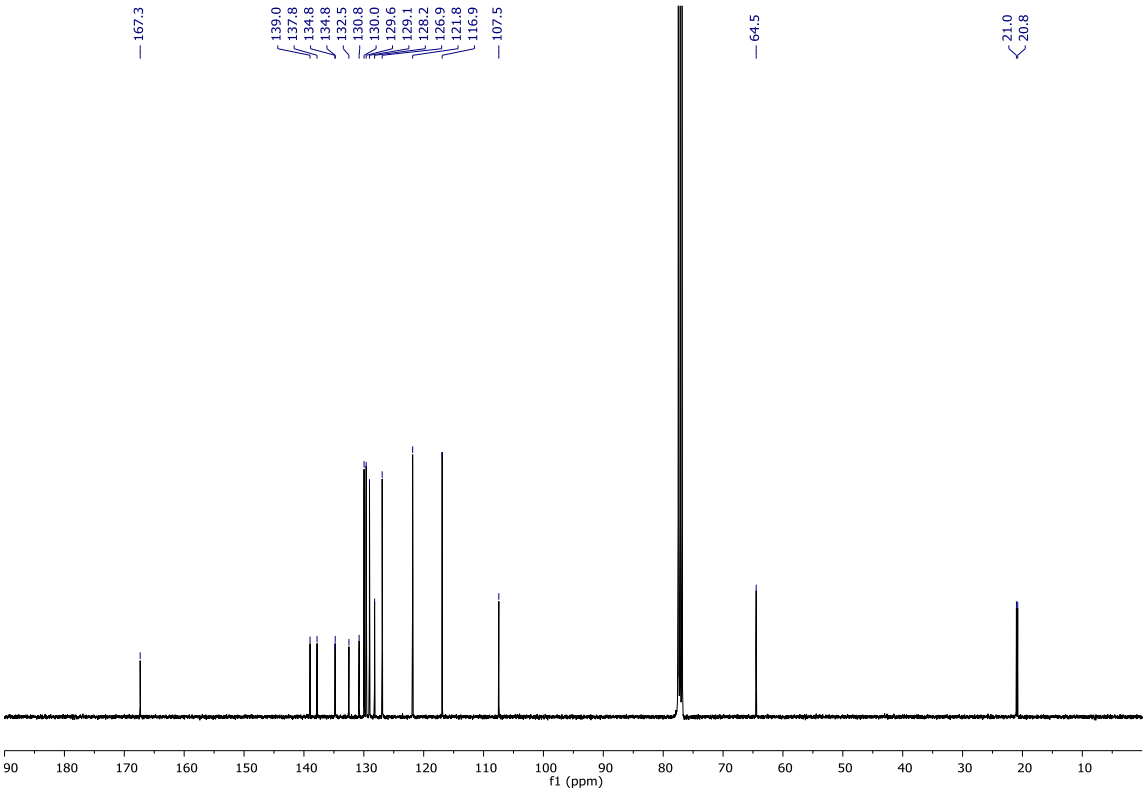


5-Phenyl-1-(*p*-tolyl)-3-(*p*-tolylamino)-1,5-dihydro-2*H*-pyrrol-2-one (1d).

^{1}H NMR (400 MHz, $CDCl_3$)

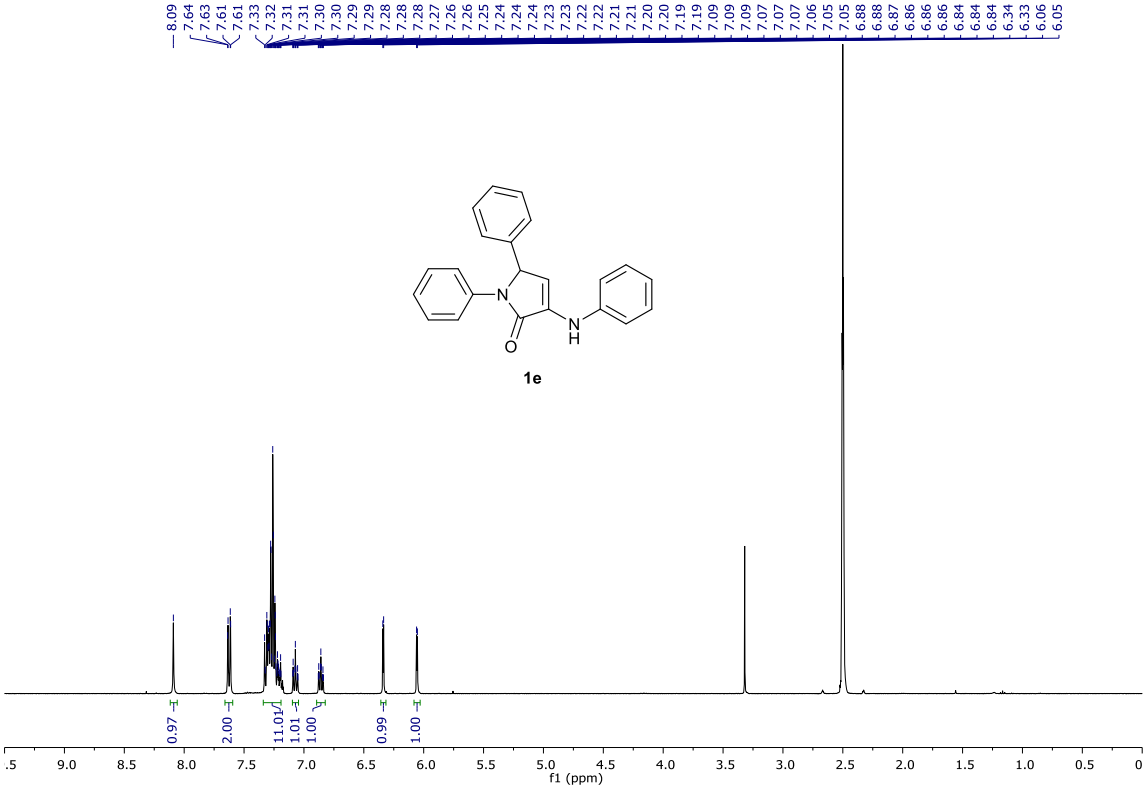


^{13}C NMR {^{1}H} (101 MHz, $CDCl_3$)

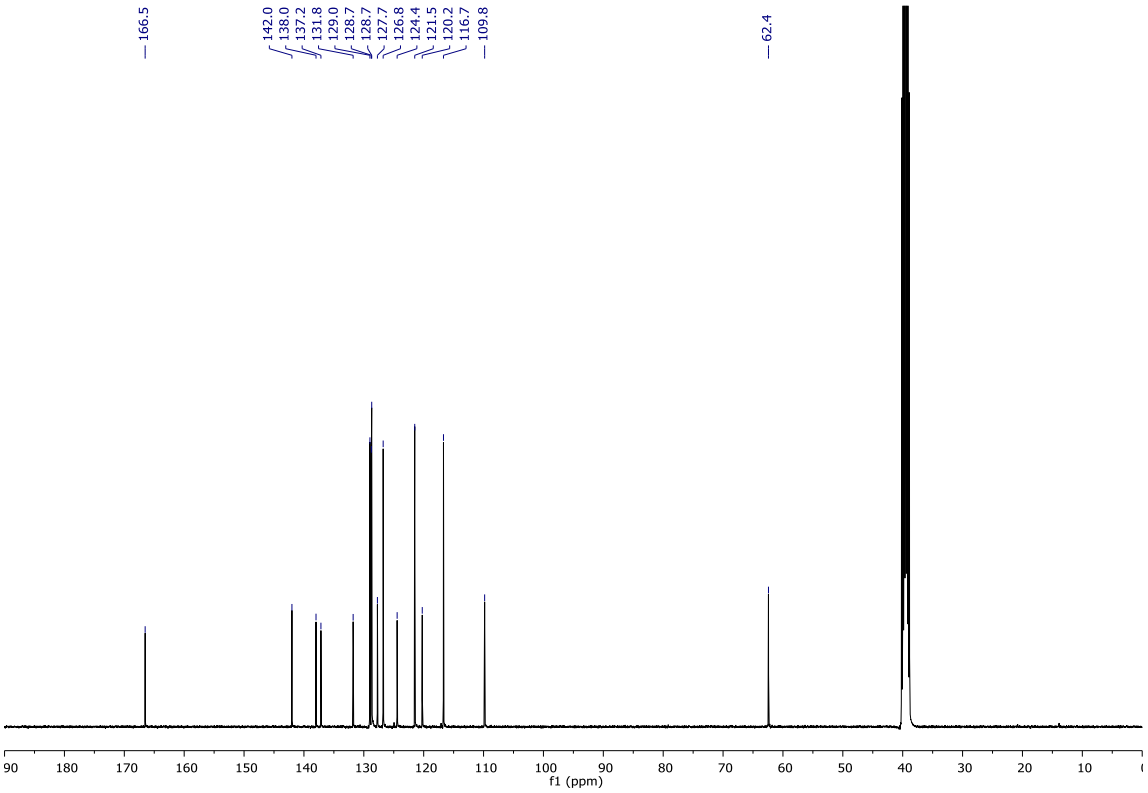


1,5-Diphenyl-3-(phenylamino)-1,5-dihydro-2*H*-pyrrol-2-one (1e)

^{1}H NMR (400 MHz, $CDCl_3$)

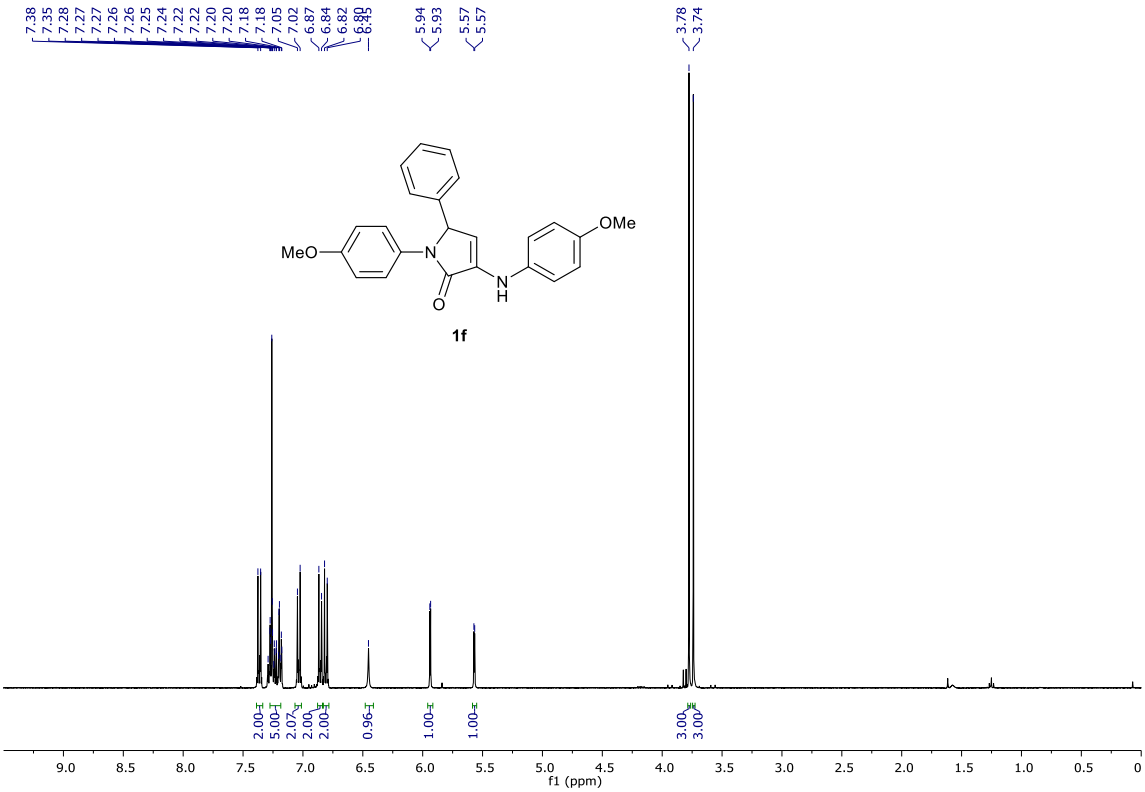


^{13}C NMR {^{1}H} (101 MHz, $CDCl_3$)

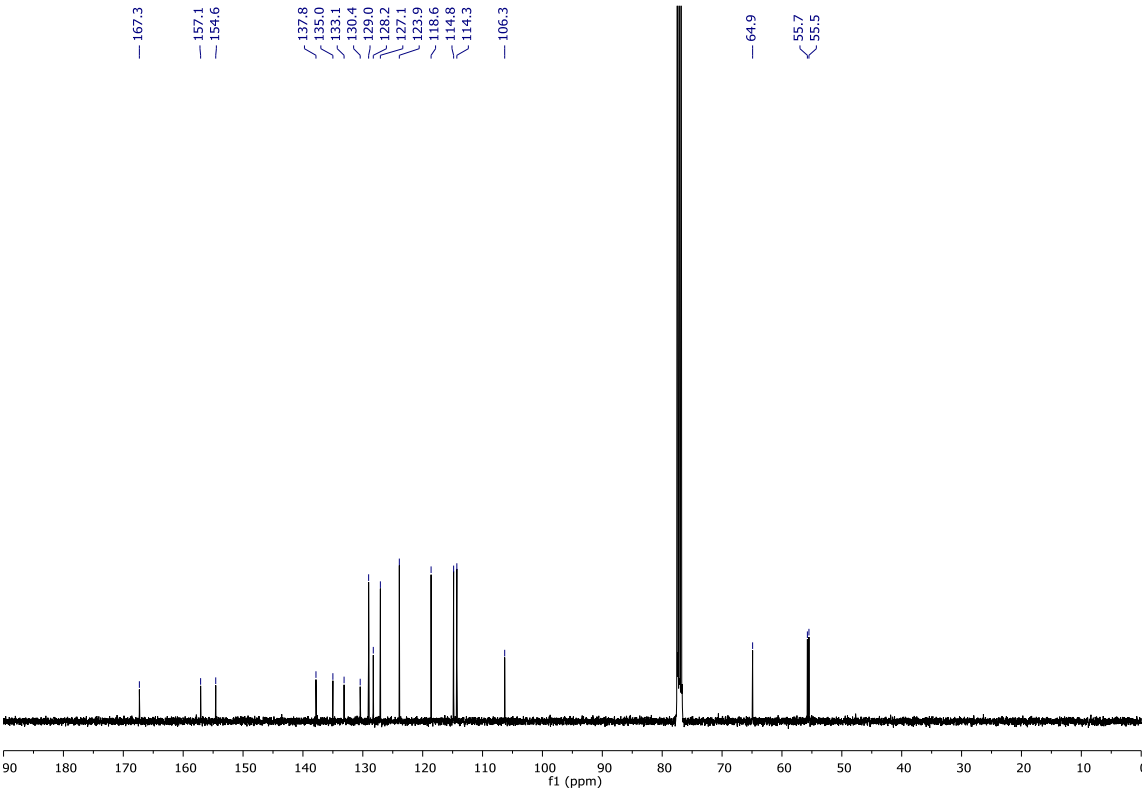


1-(4-Methoxyphenyl)-3-((4-methoxyphenyl)amino)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (1f)

^{1}H NMR (300 MHz, $CDCl_3$)

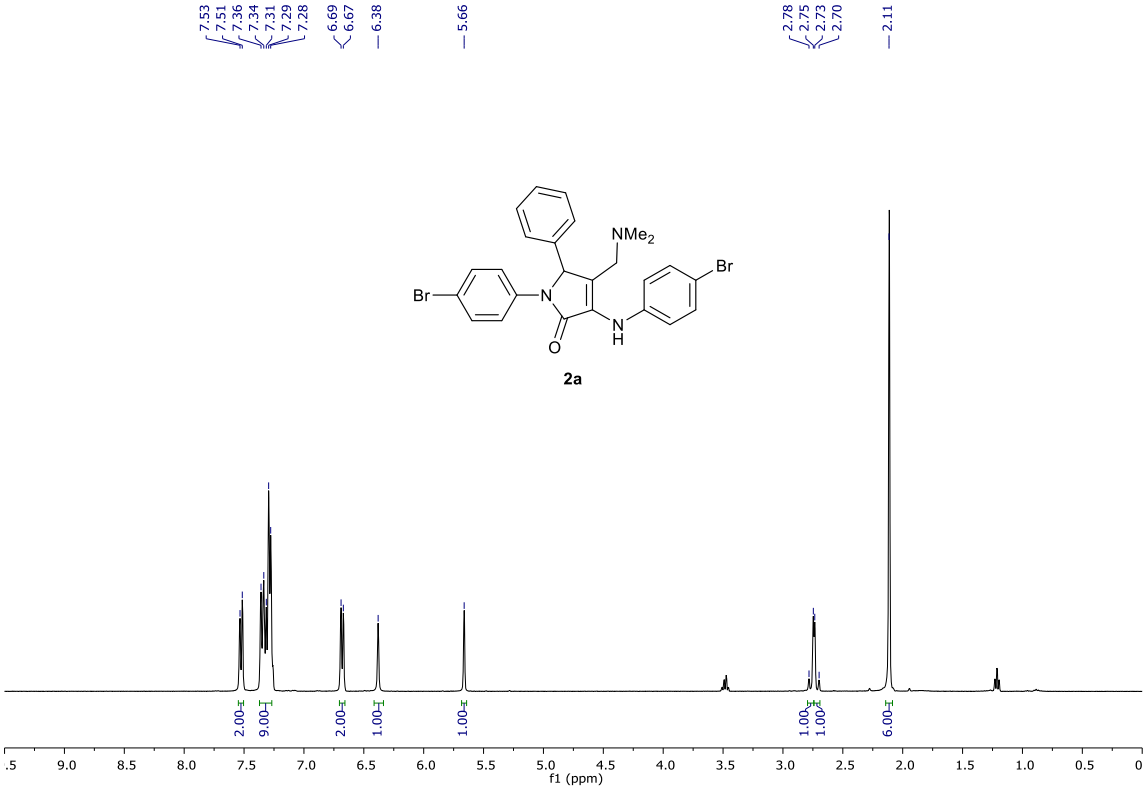


^{13}C NMR {^{1}H} (75 MHz, $CDCl_3$)

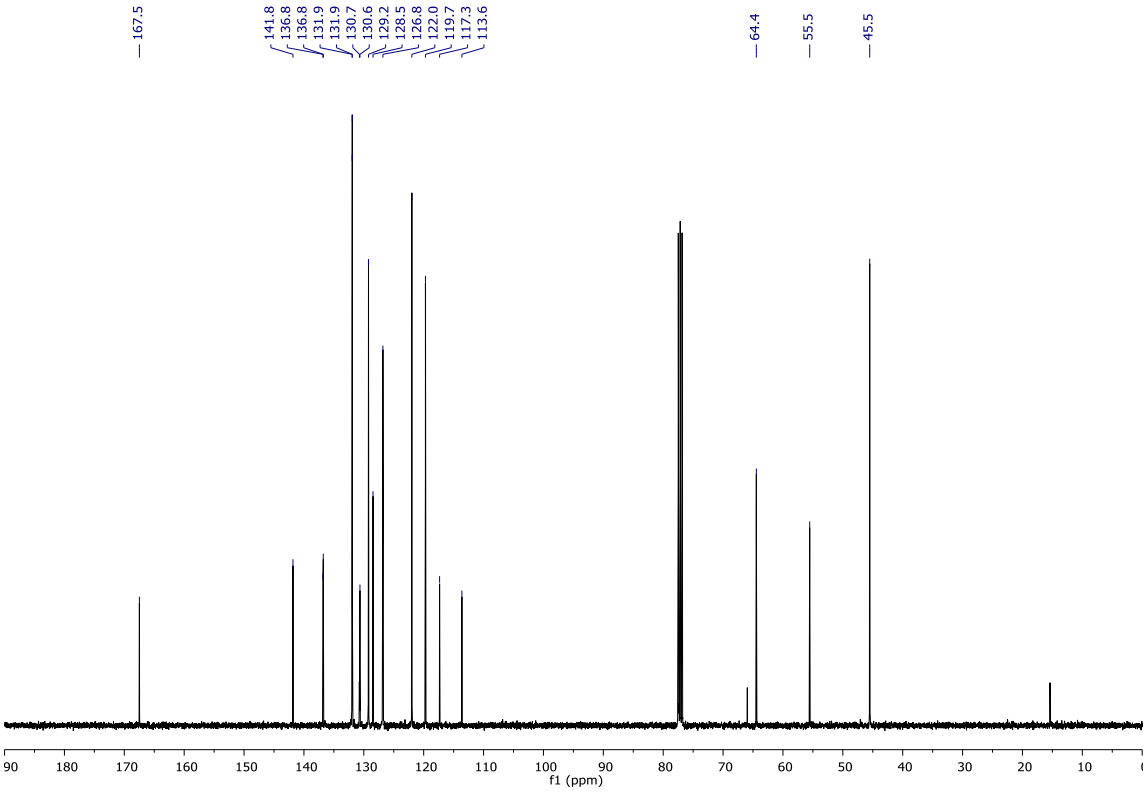


1-(4-Bromophenyl)-3-((4-bromophenyl)amino)-4-((dimethylamino)methyl)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (2a)

^{1}H NMR (400 MHz, $CDCl_3$)

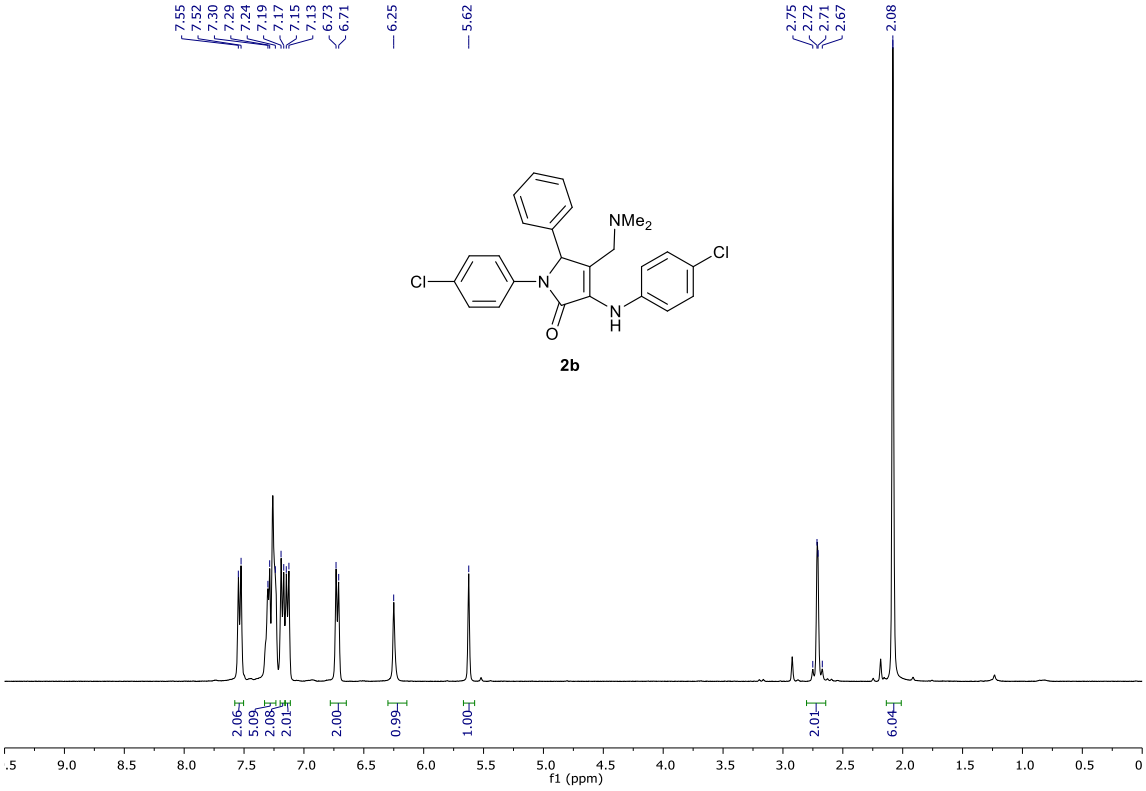


^{13}C NMR {^{1}H} (101 MHz, $CDCl_3$)

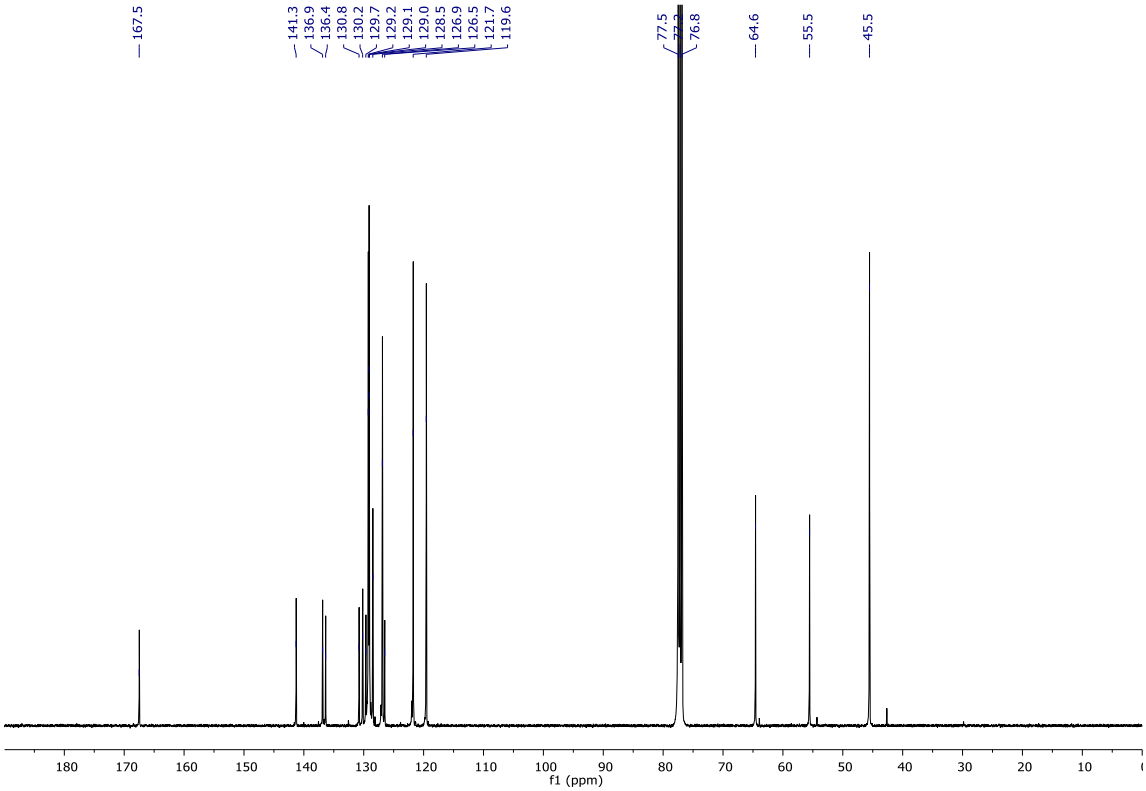


1-(4-Chlorophenyl)-3-((4-chlorophenyl)amino)-4-((dimethylamino)methyl)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (2b)

^{1}H NMR (400 MHz, $CDCl_3$)

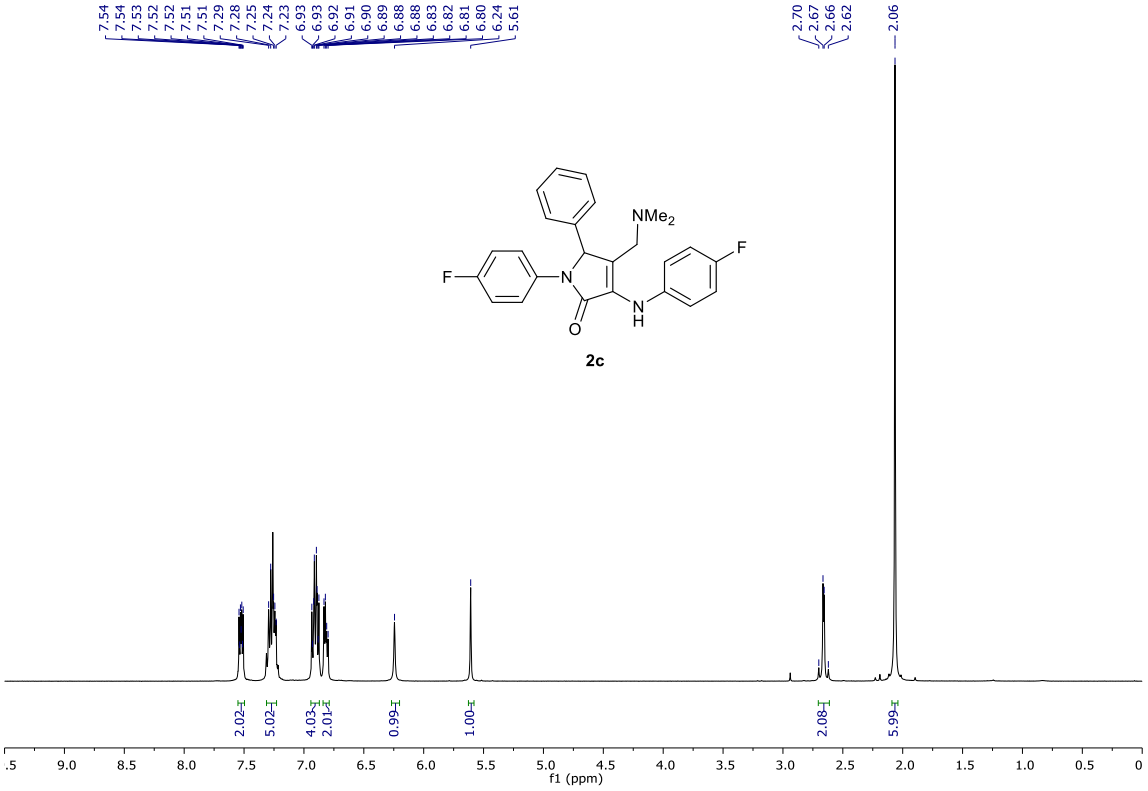


^{13}C NMR{^{1}H} (101 MHz, $CDCl_3$)

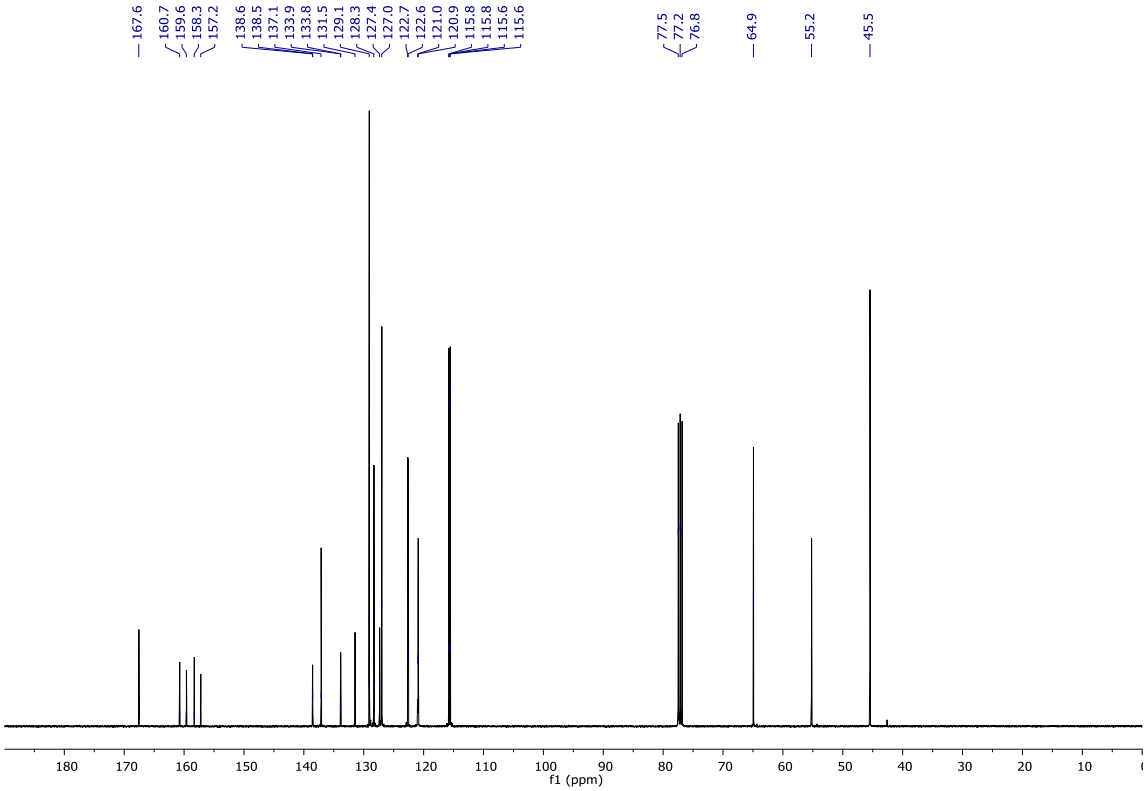


4-((Dimethylamino)methyl)-1-(4-fluorophenyl)-3-((4-fluorophenyl)amino)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (2c)

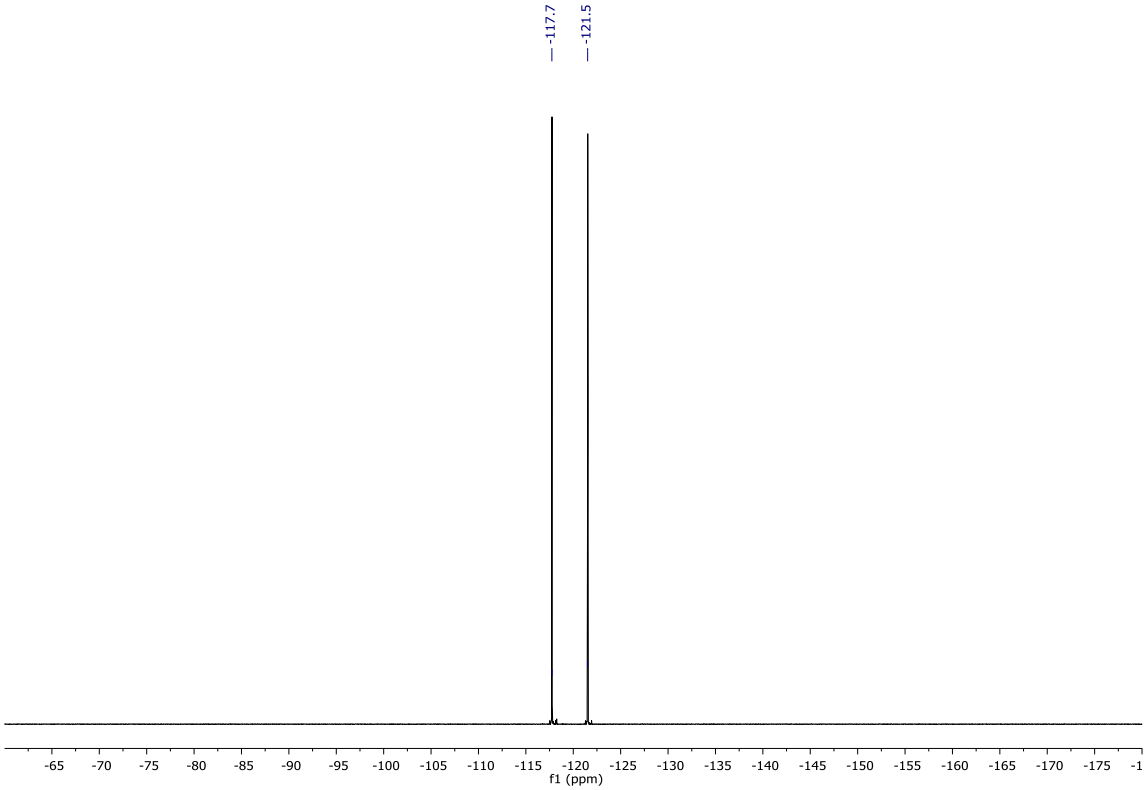
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR {^{1}H} (101 MHz, $CDCl_3$)

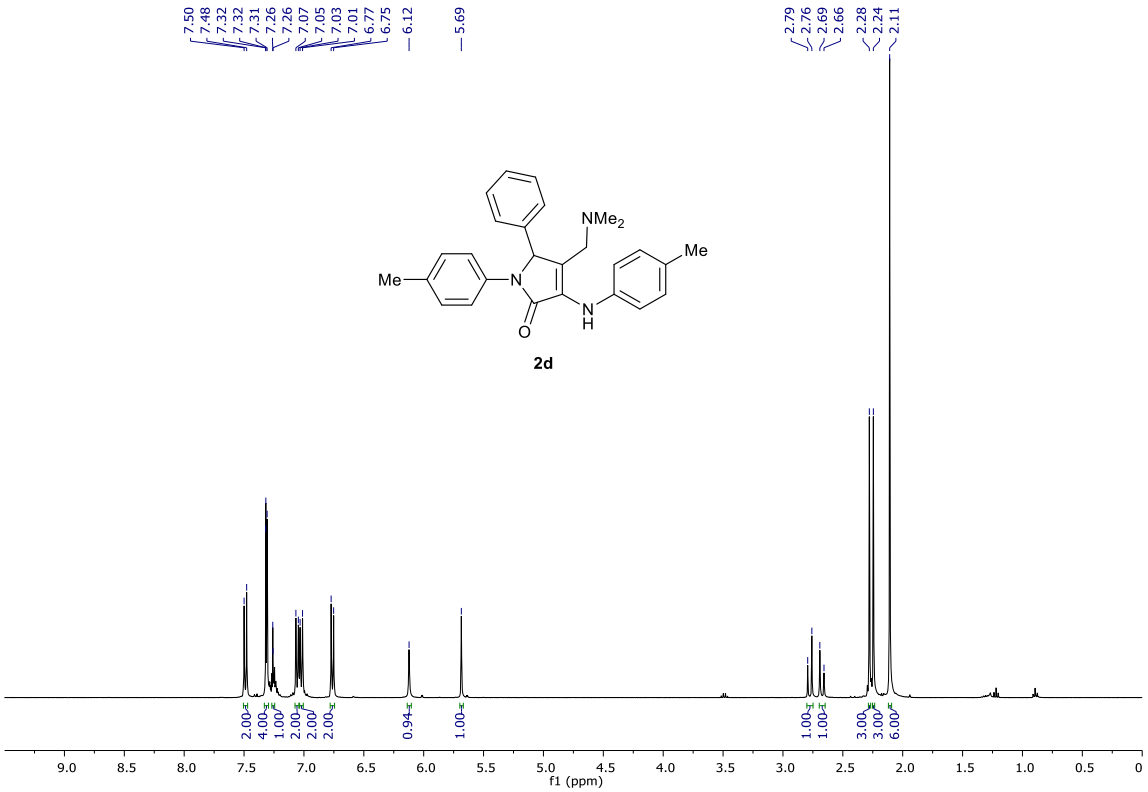


^{19}F NMR {^{1}H} (282 MHz, $CDCl_3$)

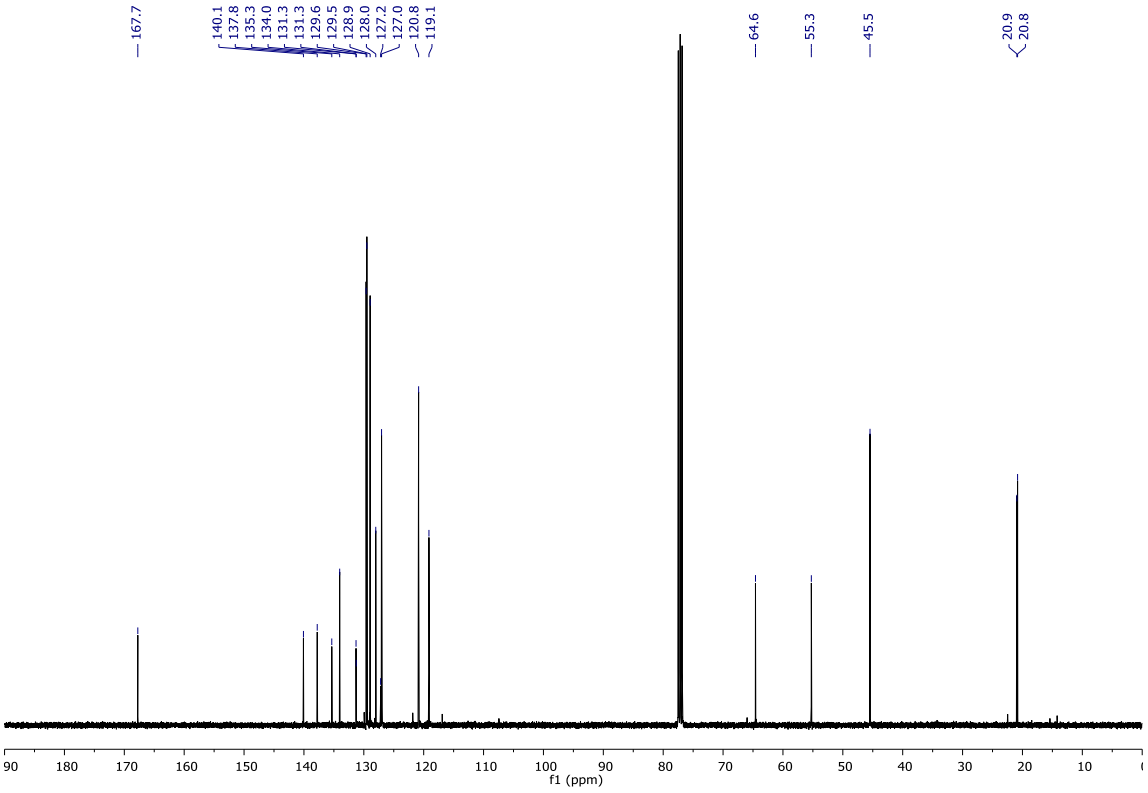


4-((Dimethylamino)methyl)-5-phenyl-1-(*p*-tolyl)-3-(*p*-tolylamino)-1,5-dihydro-2*H*-pyrrol-2-one (2d)

^{1}H NMR (400 MHz, $CDCl_3$)

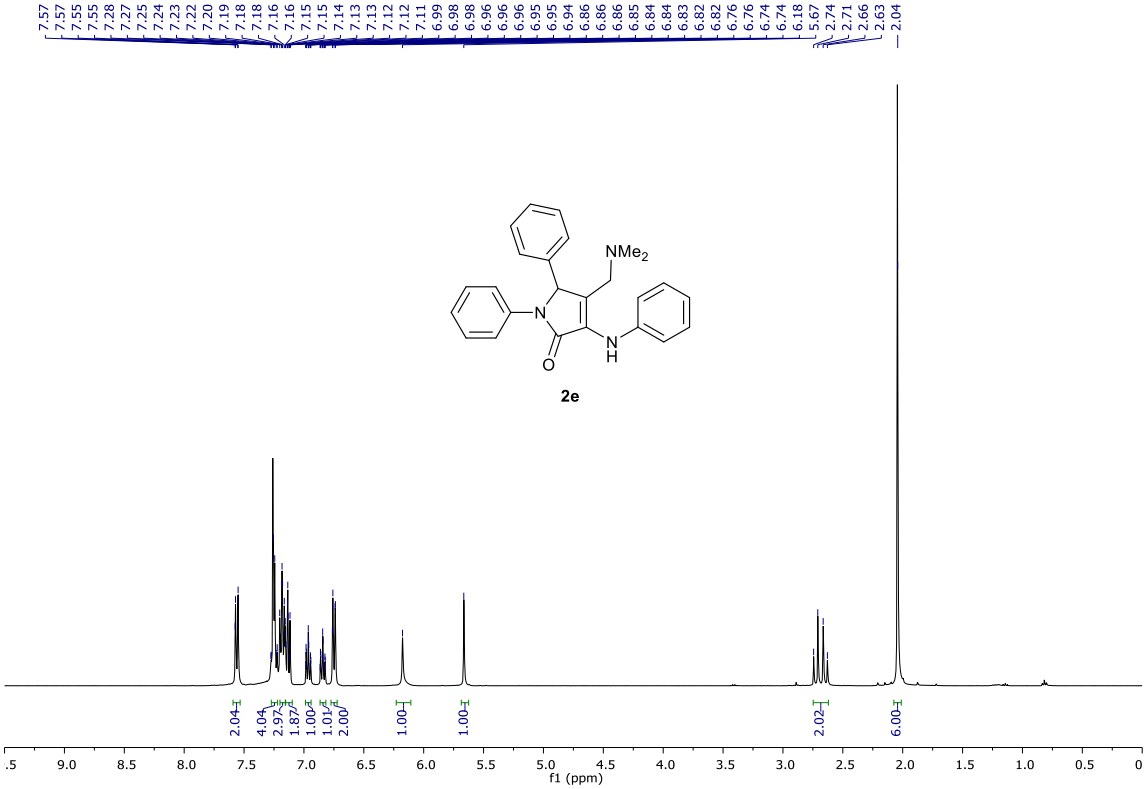


^{13}C NMR {^{1}H} (101 MHz, $CDCl_3$)

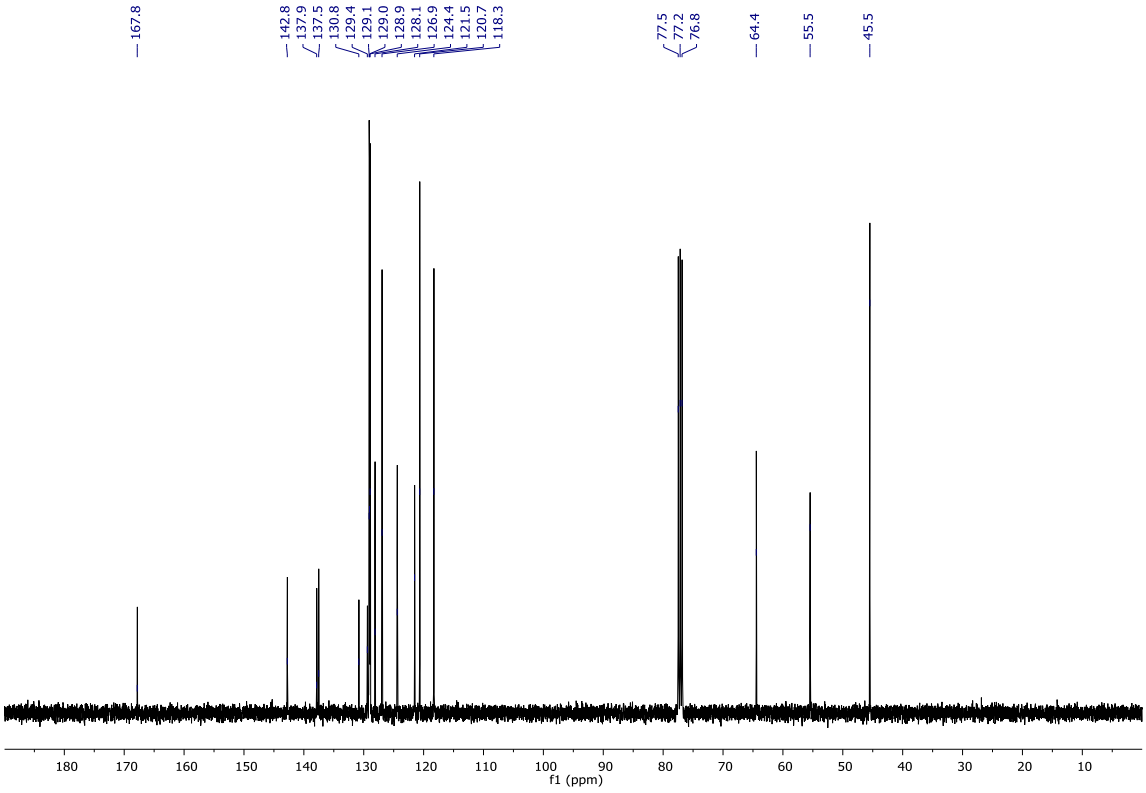


4-((dimethylamino)methyl)-1,5-diphenyl-3-(phenylamino)-1,5-dihydro-2*H*-pyrrol-2-one (2e)

^{1}H NMR (400 MHz, $CDCl_3$)

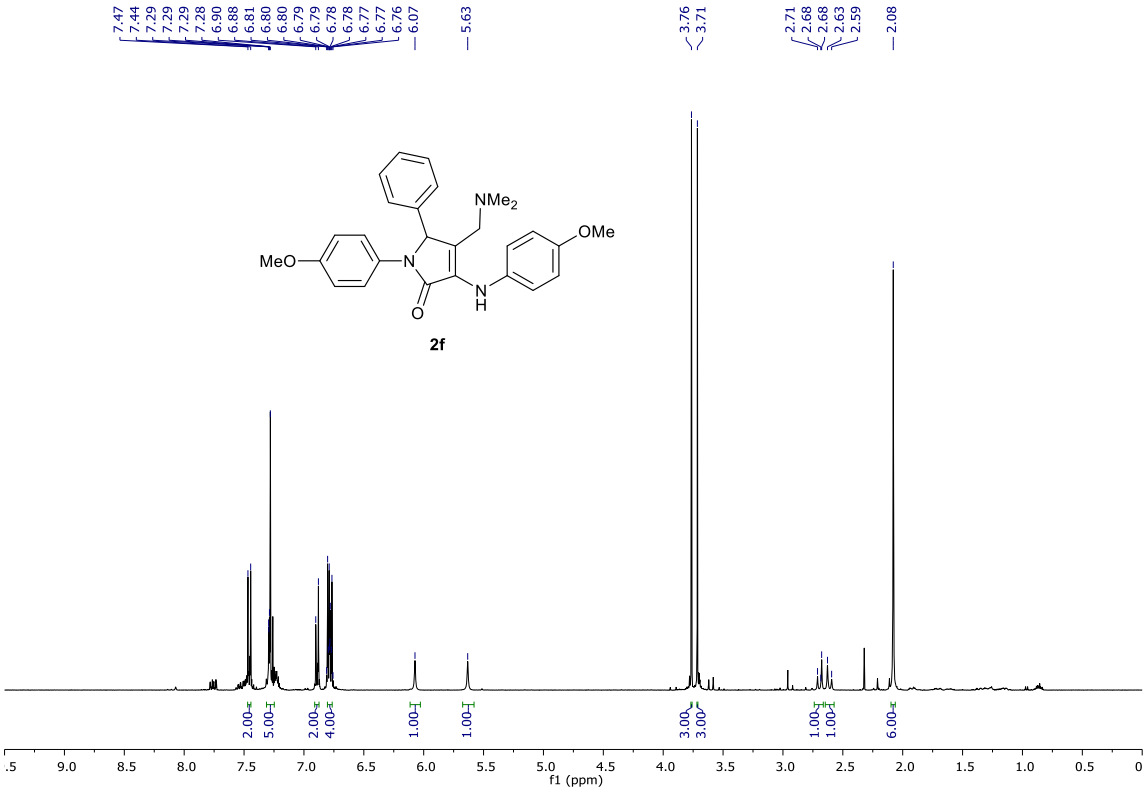


^{13}C NMR {^{1}H} (101 MHz, $CDCl_3$)

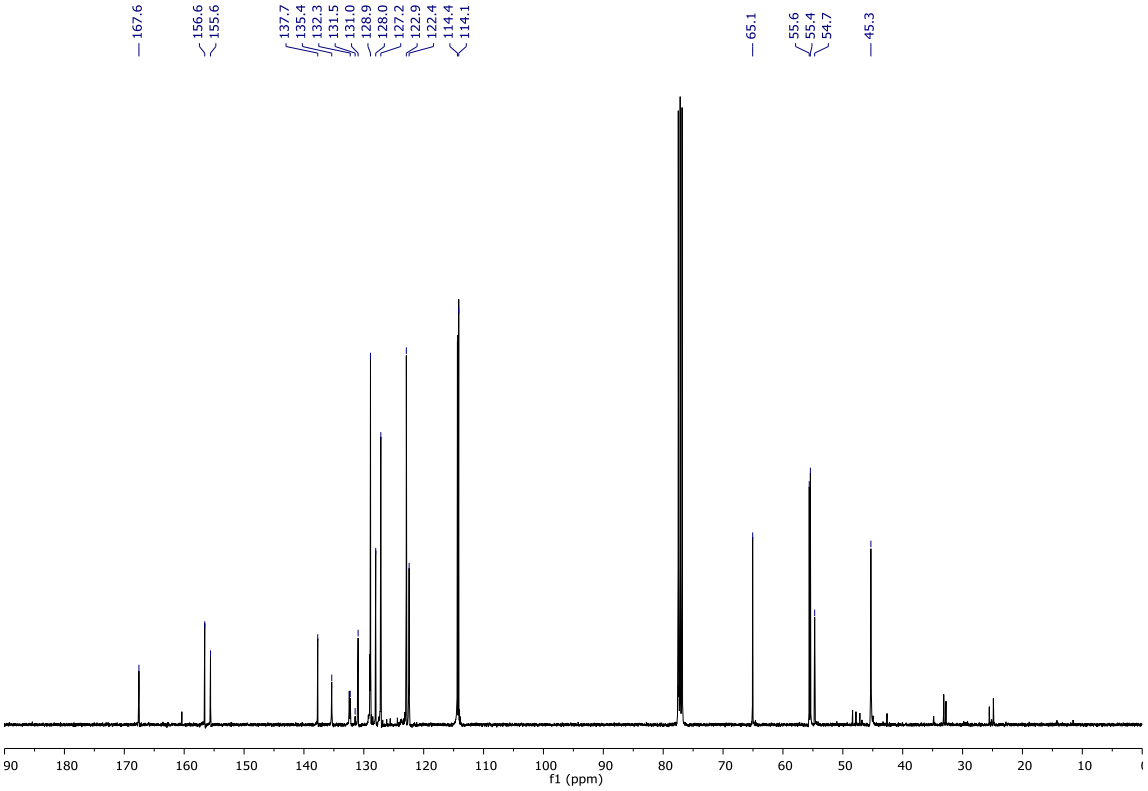


4-((Dimethylamino)methyl)-1-(4-methoxyphenyl)-3-((4-methoxyphenyl)amino)-5-phenyl-1,5-dihydro-2*H*-pyrrol-2-one (2f)

^{1}H NMR (400 MHz, $CDCl_3$)

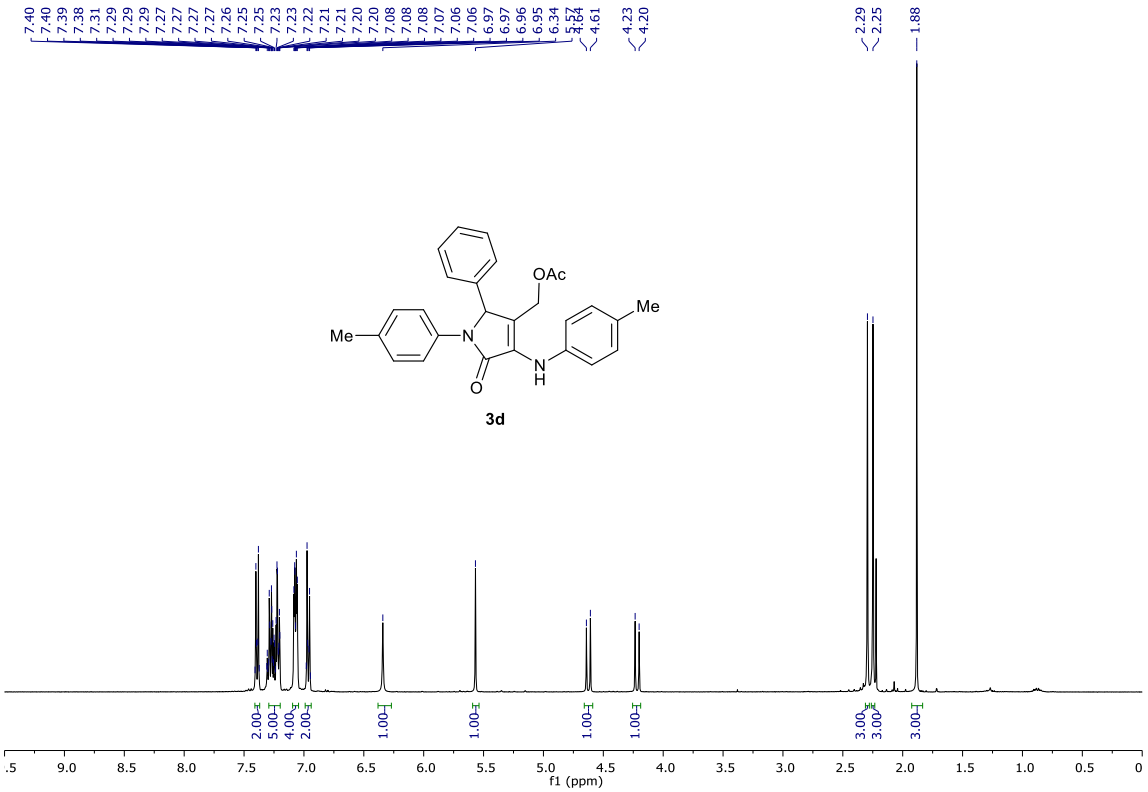


^{13}C NMR {^{1}H} (101 MHz, $CDCl_3$)

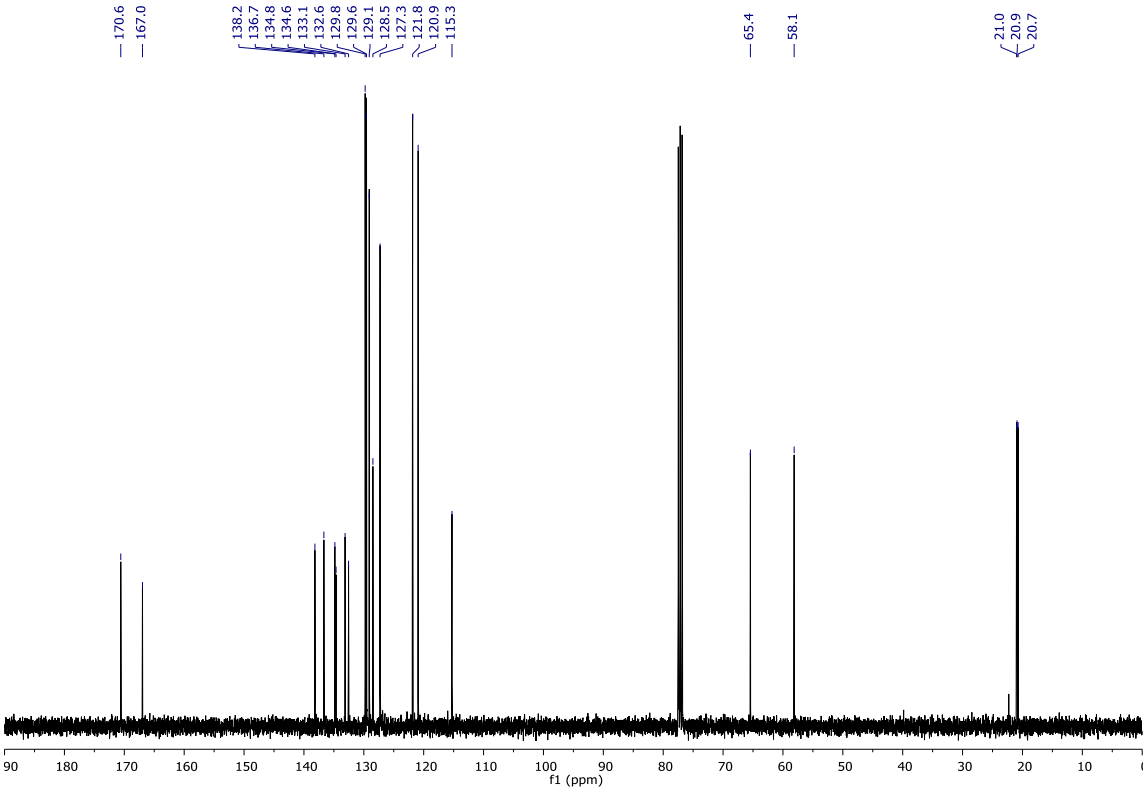


(5-Oxo-2-phenyl-1-(*p*-tolyl)-4-(*p*-tolylamino)-2,5-dihydro-1*H*-pyrrol-3-yl)methyl acetate (3d)

^{1}H NMR (400 MHz, $CDCl_3$)

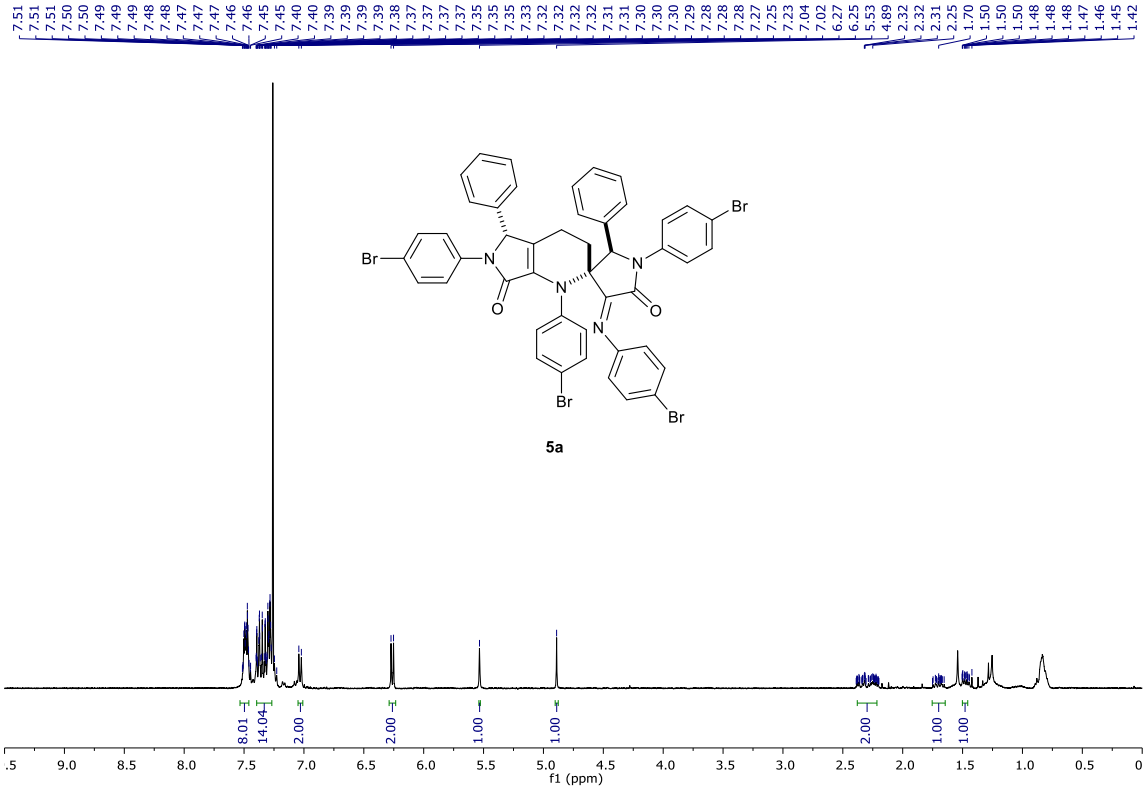


^{13}C NMR {^{1}H} (101 MHz, $CDCl_3$)

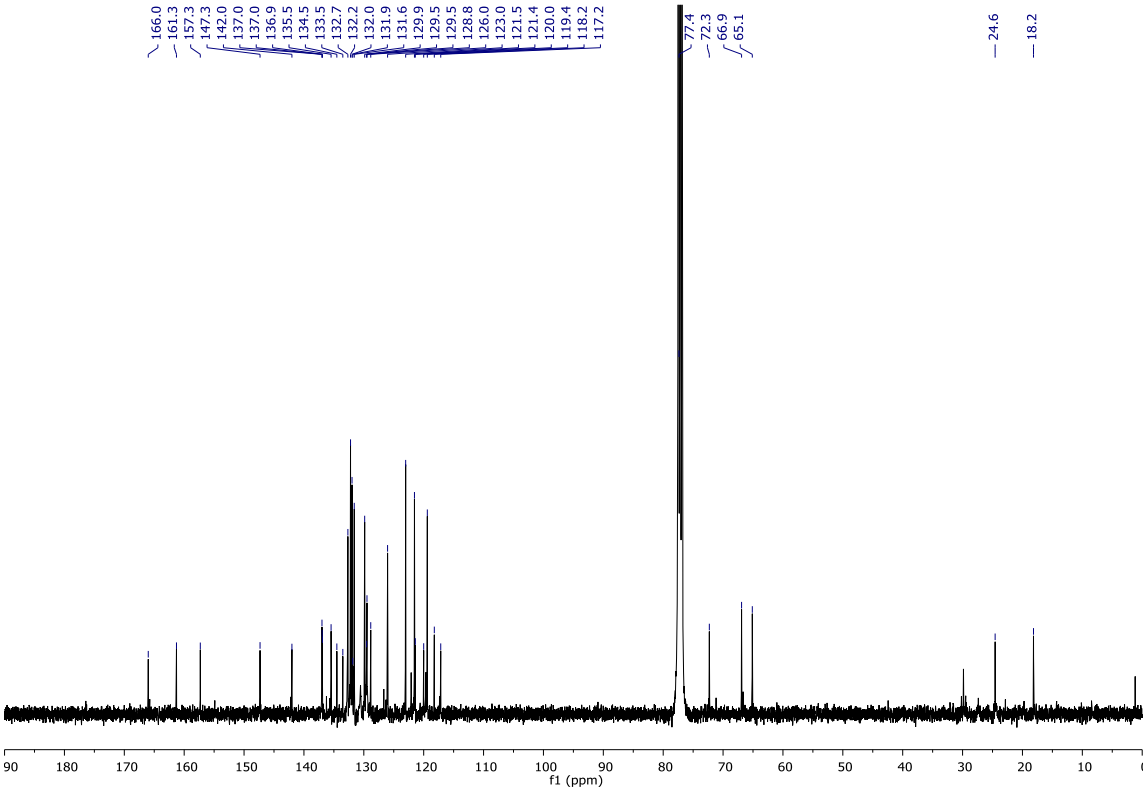


(2*R,3*R**,5'*S**,*Z*)-1,1',6'-Tris(4-bromophenyl)-4-((4-bromophenyl)imino)-2,5'-diphenyl-3',4',5',6'-tetrahydrospiro[pyrrolidine-3,2'-pyrrolo[3,4-*b*]pyridine]-5,7'(1'*H*)-dione (5a)**

^{1}H NMR (400 MHz, $CDCl_3$)

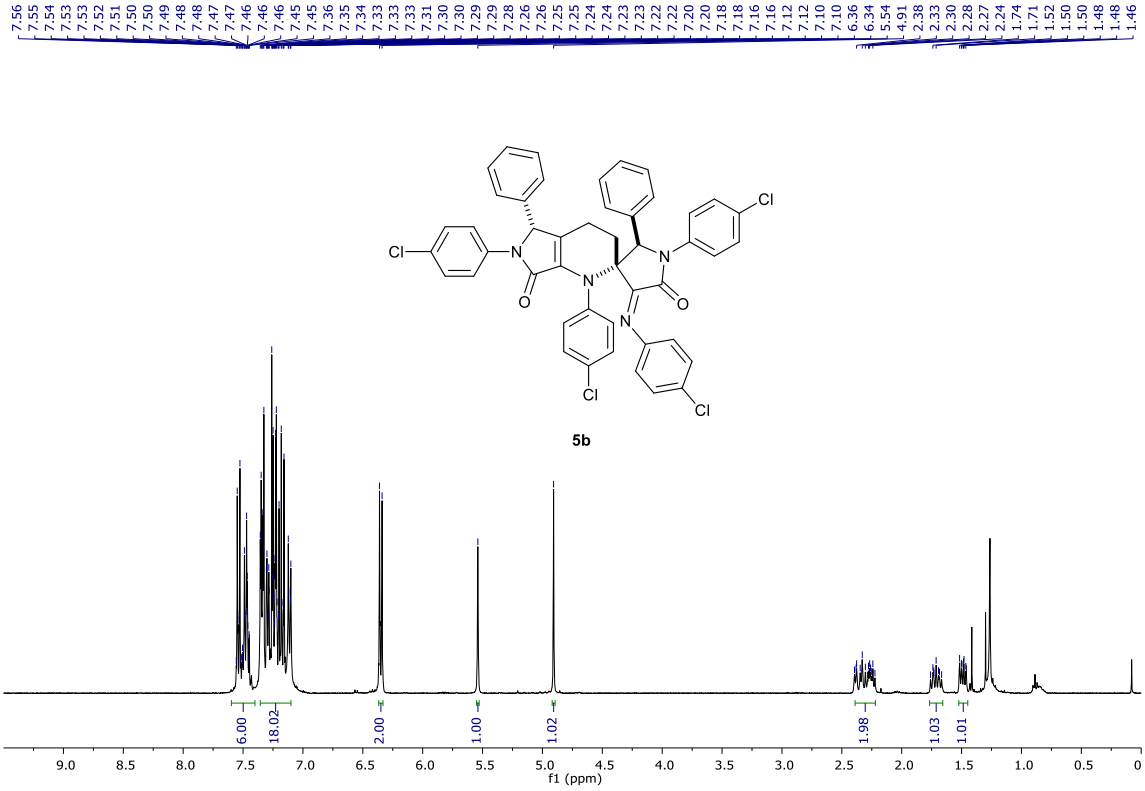


^{13}C NMR {^{1}H} (101 MHz, $CDCl_3$)

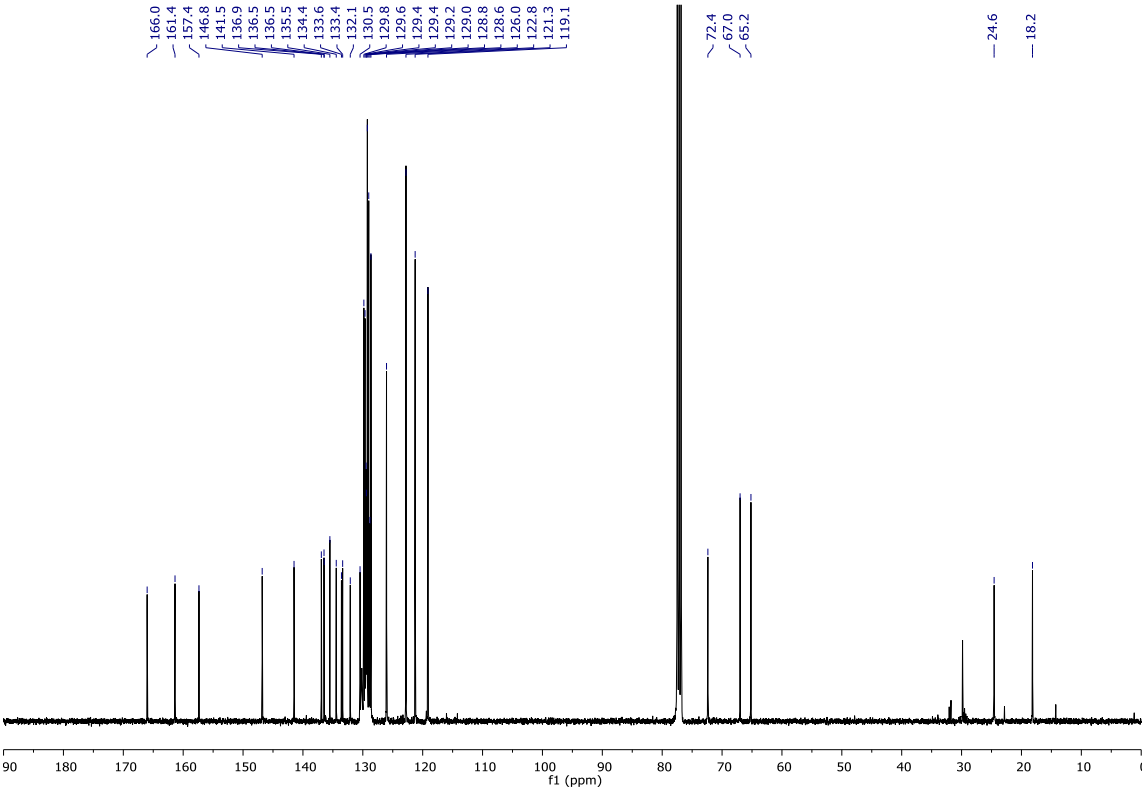


(2*R,3*R**,5'*R**,*Z*)-1,1',6'-Tris(4-chlorophenyl)-4-((4-chlorophenyl)imino)-2,5'-diphenyl-3',4',5',6'-tetrahydrospiro[pyrrolidine-3,2'-pyrrolo[3,4-*b*]pyridine]-5,7'(1'*H*)-dione (5b)**

^{1}H NMR (400 MHz, $CDCl_3$)

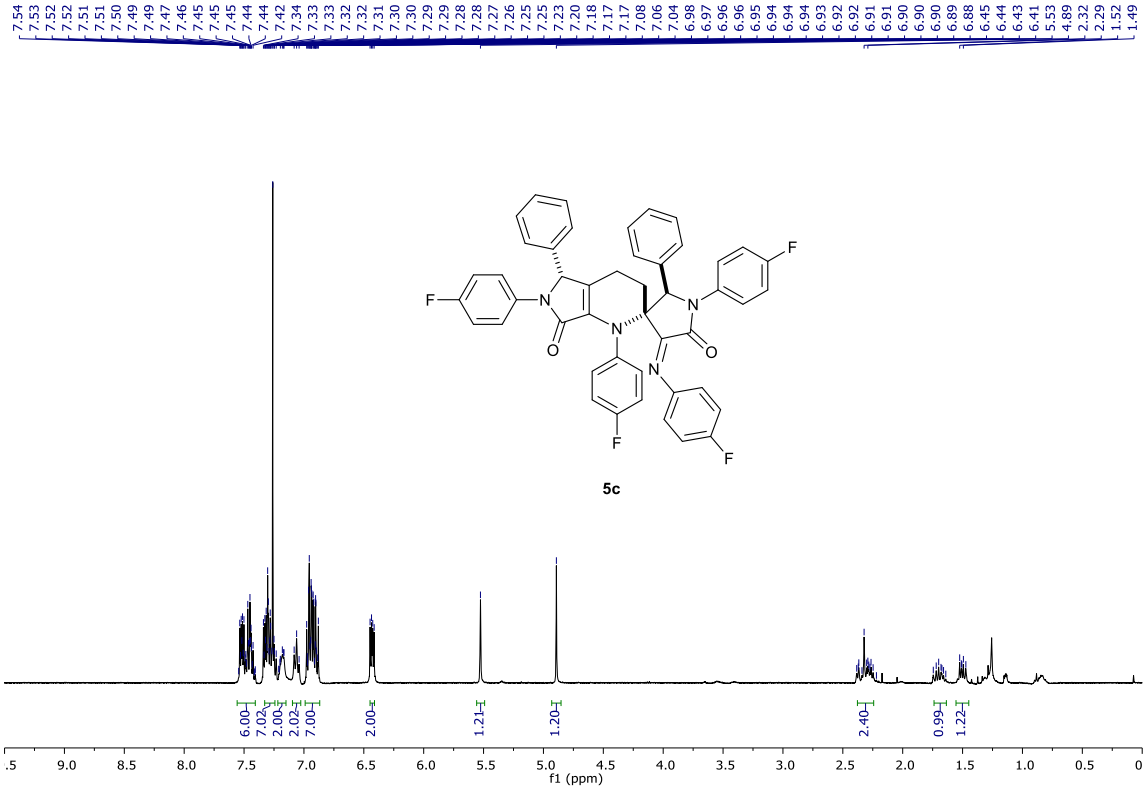


^{13}C NMR {^{1}H} (101 MHz, $CDCl_3$)

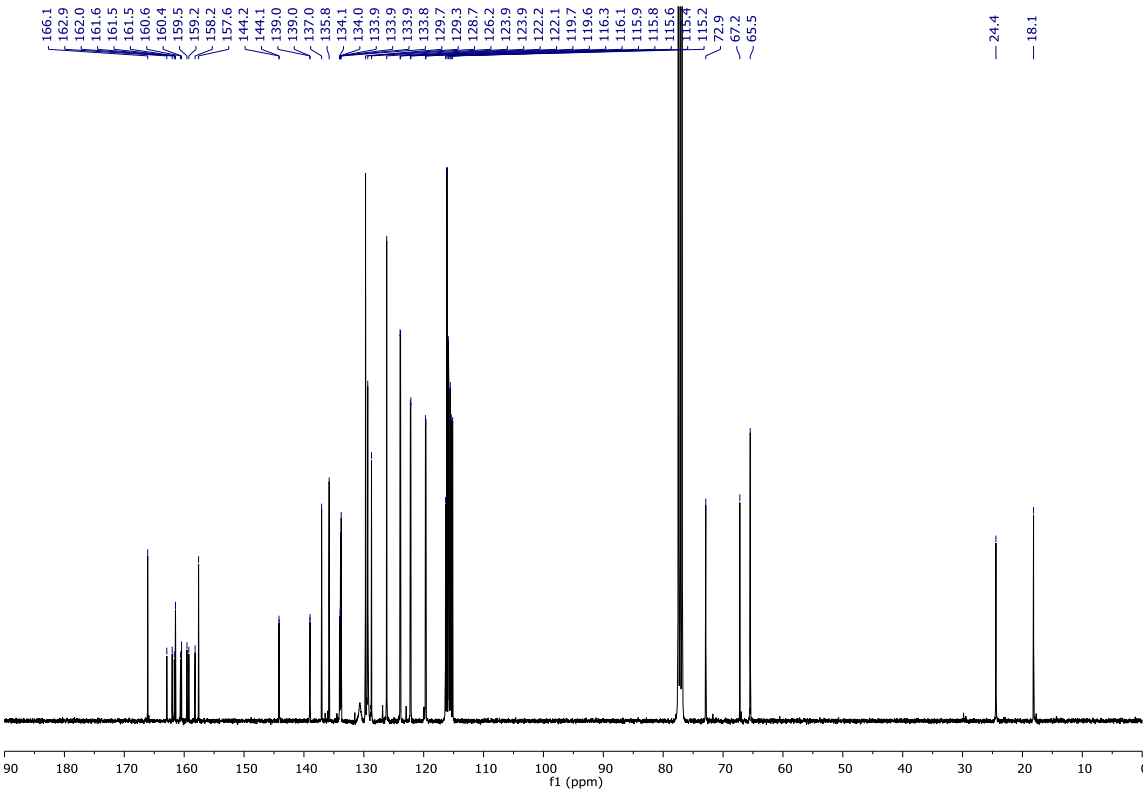


(2*R,3*R**,5'*R**,*Z*)-1,1',6'-Tris(4-fluorophenyl)-4-((4-fluorophenyl)imino)-2,5'-diphenyl-3',4',5',6'-tetrahydrospiro[pyrrolidine-3,2'-pyrrolo[3,4-*b*]pyridine]-5,7'(1'*H*)-dione (5c)**

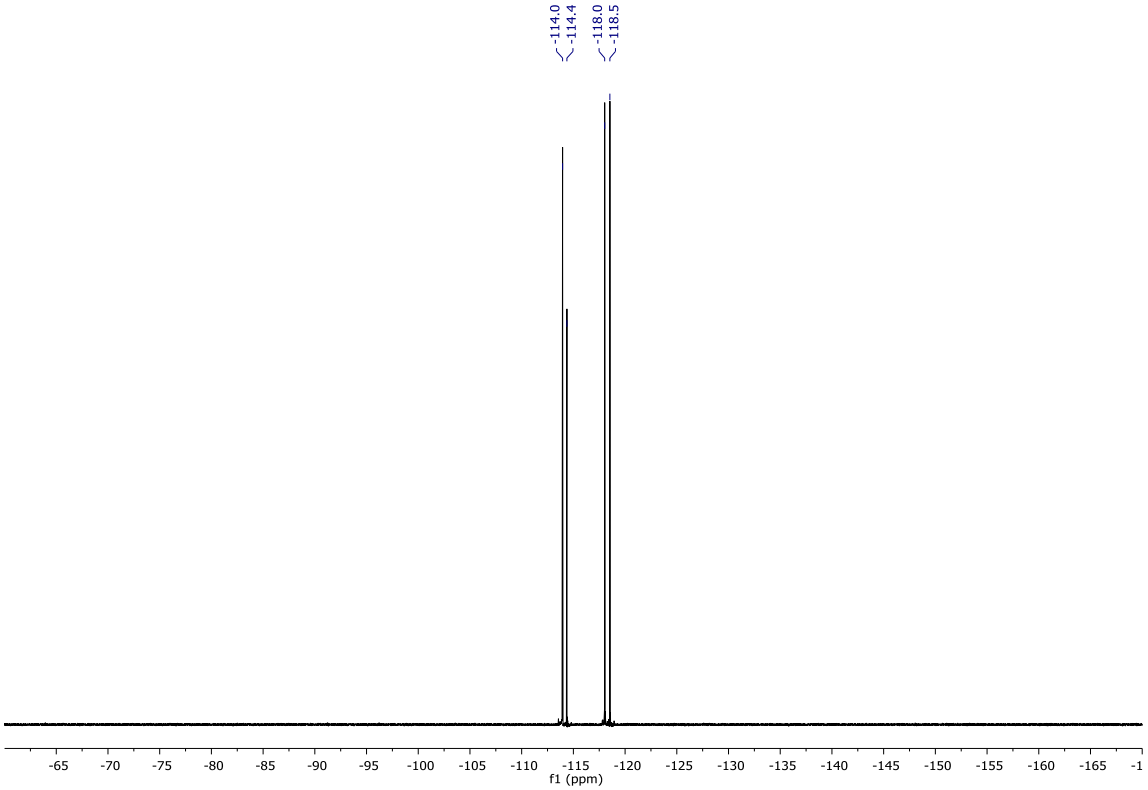
^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR{^{1}H} (101 MHz, $CDCl_3$)

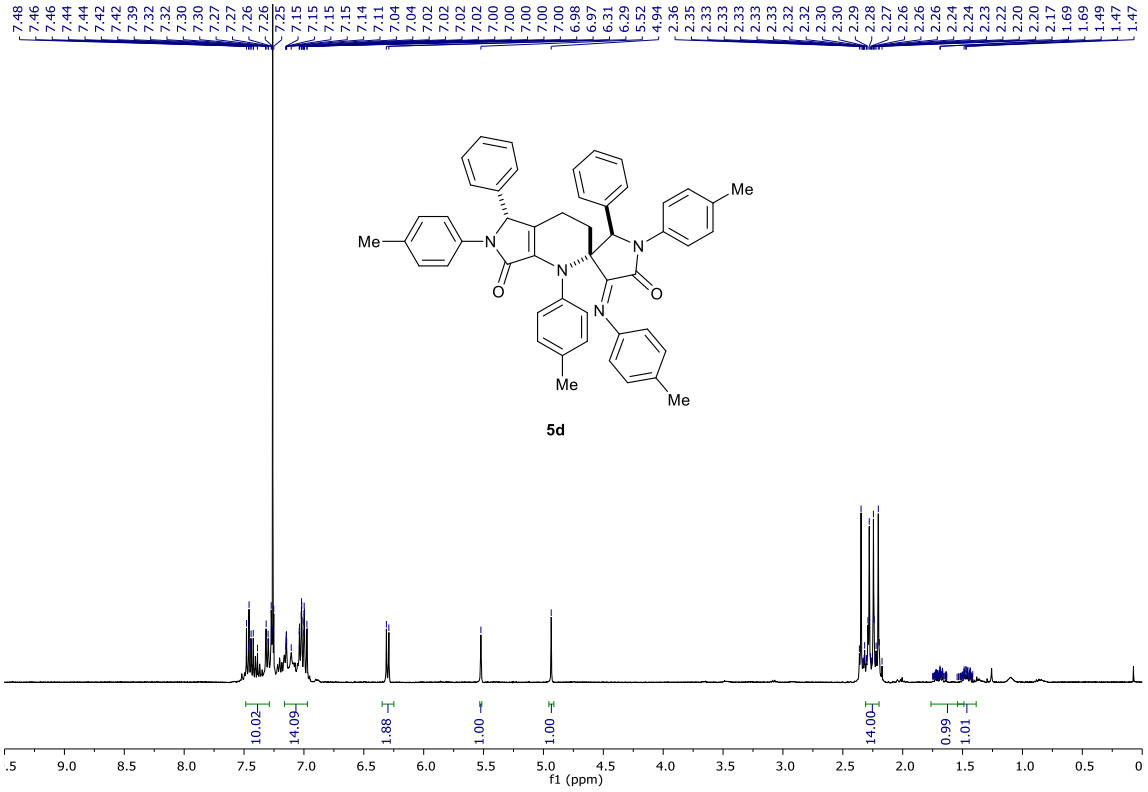


^{19}F NMR {^{1}H} (282 MHz, $CDCl_3$)

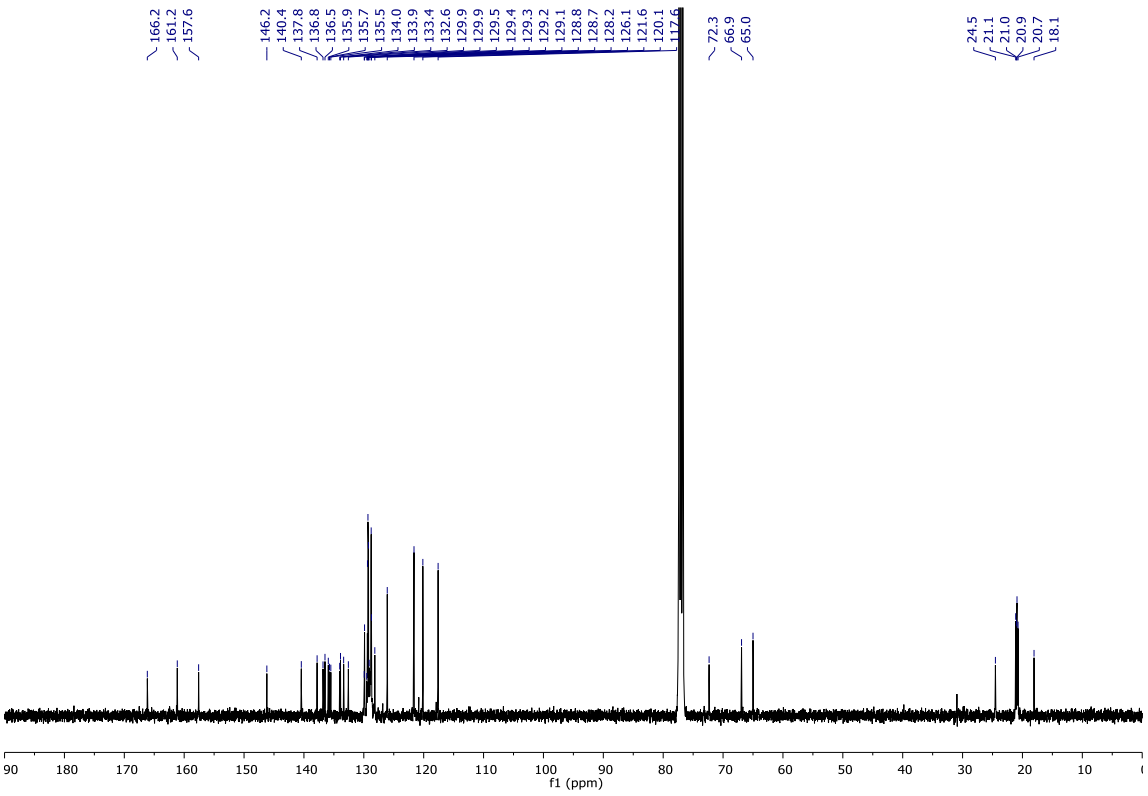


(2*R,3*R**,5'*R**,*Z*)-2,5'-Diphenyl-1,1',6'-tri-*p*-tolyl-4-(*p*-tolylimino)-3',4',5',6'-tetrahydrospiro[pyrrolidine-3,2'-pyrrolo[3,4-*b*]pyridine]-5,7'(1'*H*)-dione (5d)**

^{1}H NMR (400 MHz, $CDCl_3$)

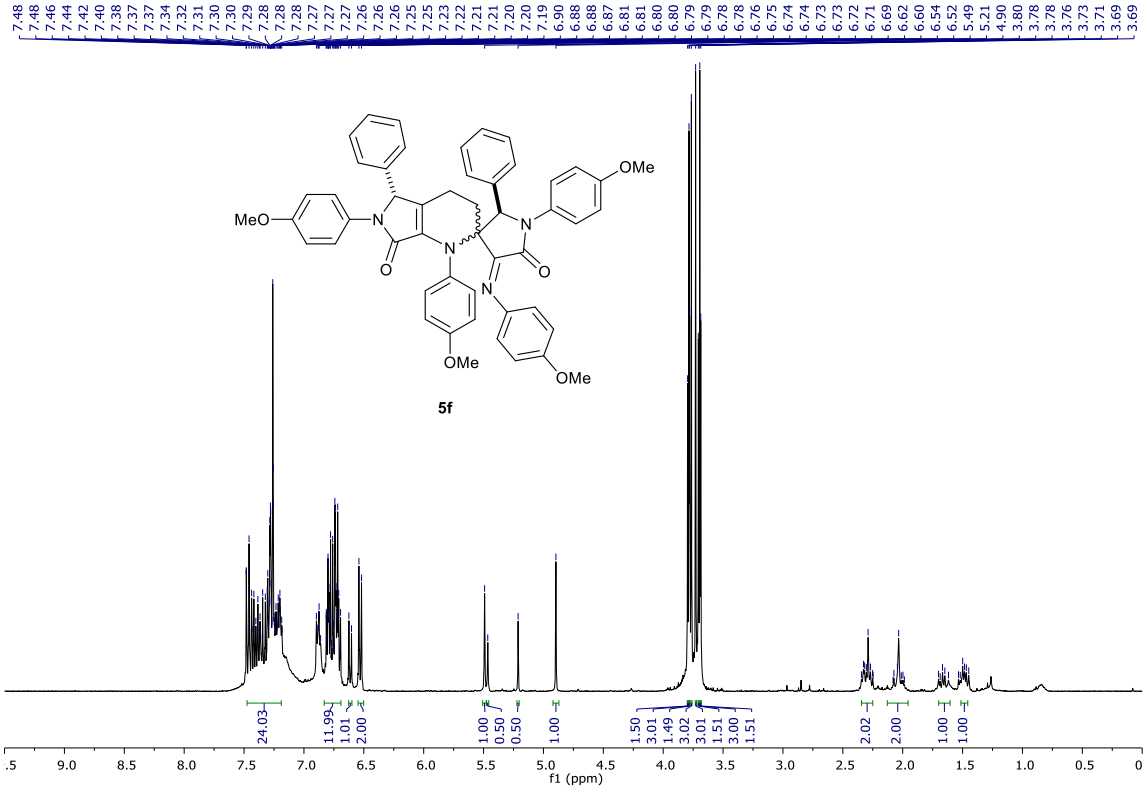


^{13}C NMR {^{1}H} (101 MHz, $CDCl_3$)

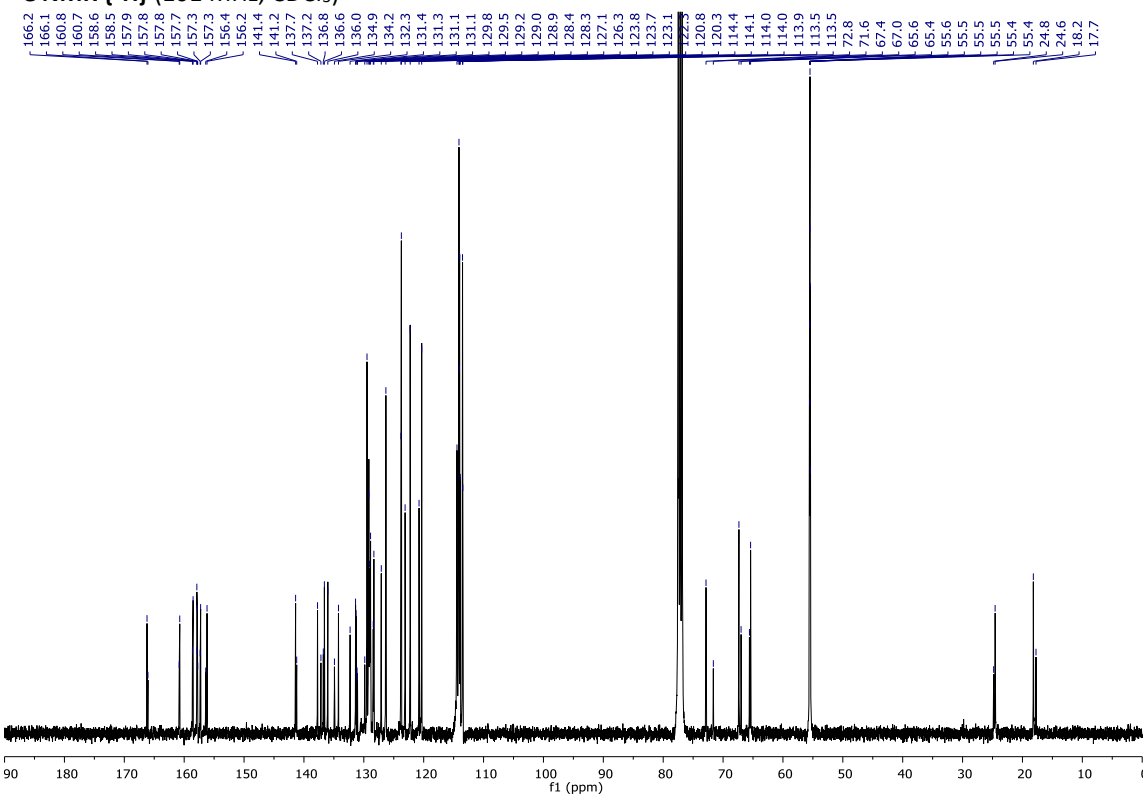


(2*R,5'*R**,Z)-1,1',6'-Tris(4-methoxyphenyl)-4-((4-methoxyphenyl)imino)-2,5'-diphenyl-3',4',5',6'-tetrahydrospiro[pyrrolidine-3,2'-pyrrolo[3,4-*b*]pyridine]-5,7'(1'*H*)-dione (5f)**

^{1}H NMR (400 MHz, $CDCl_3$)



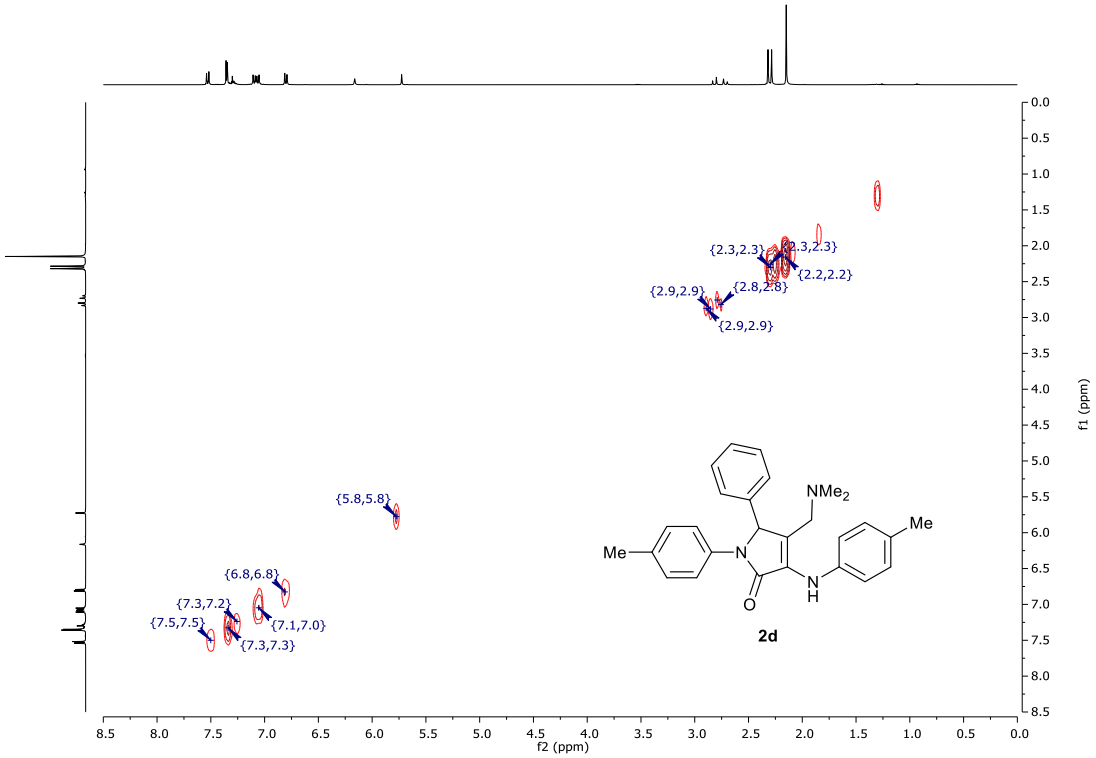
^{13}C NMR {^{1}H} (101 MHz, $CDCl_3$)



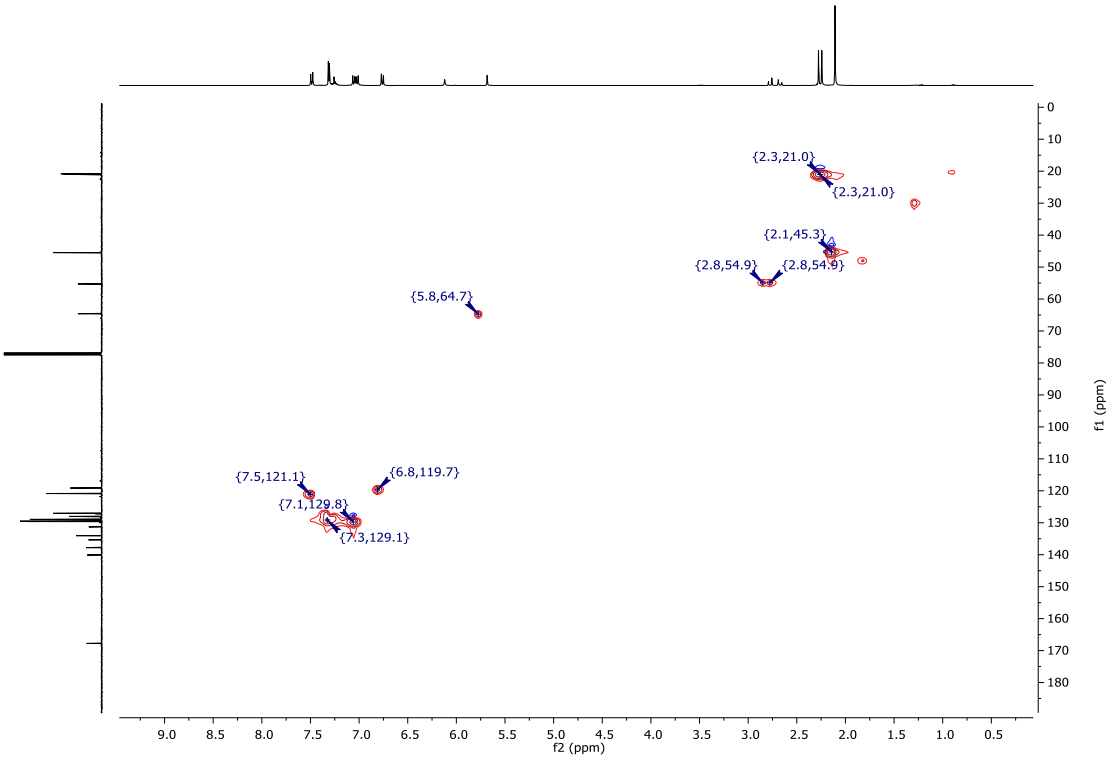
VI. Copies of 2D NMR spectra for 2d and 5b

4-((Dimethylamino)methyl)-5-phenyl-1-(*p*-tolyl)-3-(*p*-tolylamino)-1,5-dihydro-2*H*-pyrrol-2-one (2d).

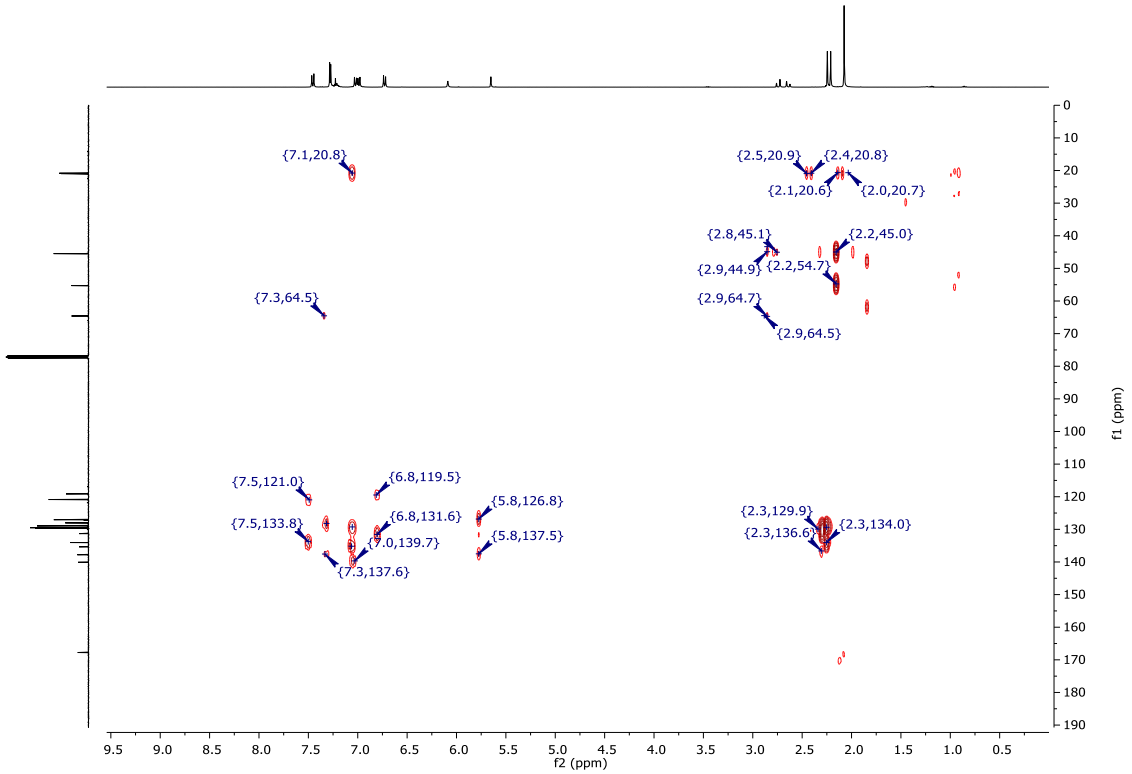
2D-COSY NMR {^{1}H – ^{1}H} (400 MHz, $CDCl_3$)



2D-HSQC NMR {^{1}H – ^{13}C} (^{1}H: 400 MHz, ^{13}C: 101 MHz, $CDCl_3$)

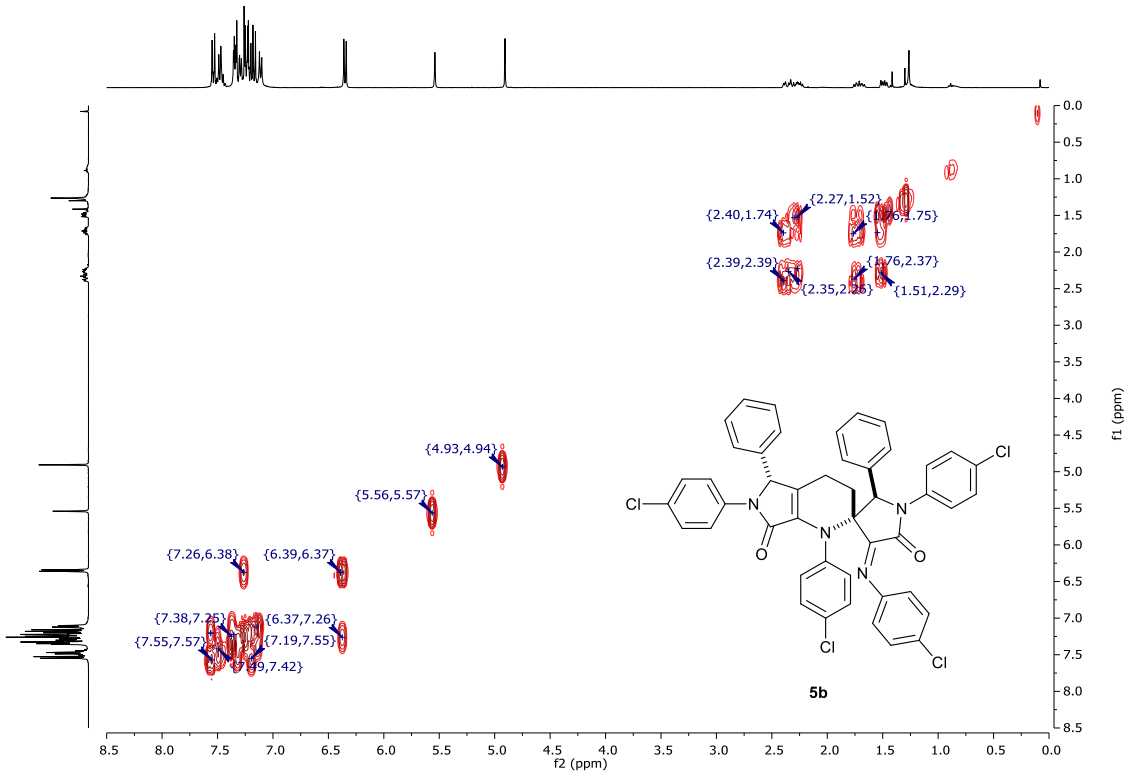


2D-HMBC NMR {^{1}H – ^{13}C} (^{1}H: 400 MHz, ^{13}C: 101 MHz, $CDCl_3$)

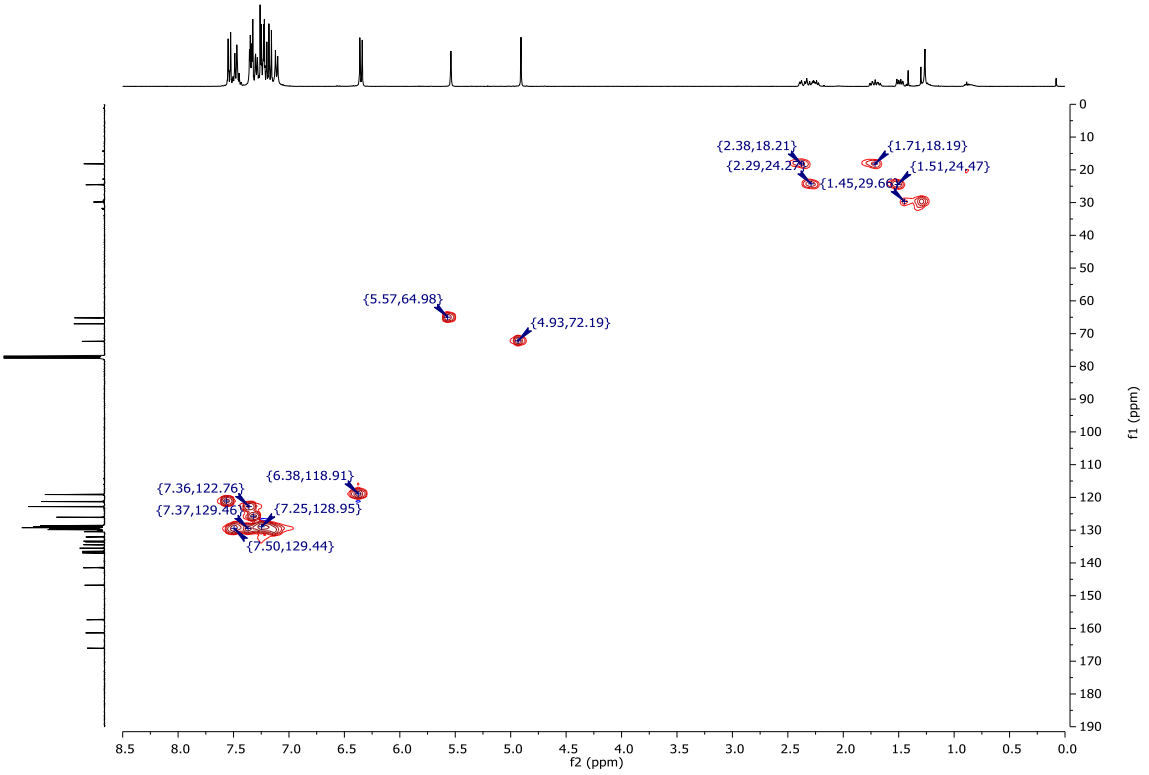


(2*R,3*R**,5'*R**,*Z*)-1,1',6'-Tris(4-chlorophenyl)-4-((4-chlorophenyl)imino)-2,5'-diphenyl-3',4',5',6'-tetrahydrospiro[pyrrolidine-3,2'-pyrrolo[3,4-*b*]pyridine]-5,7'(1'*H*)-dione (5b)**

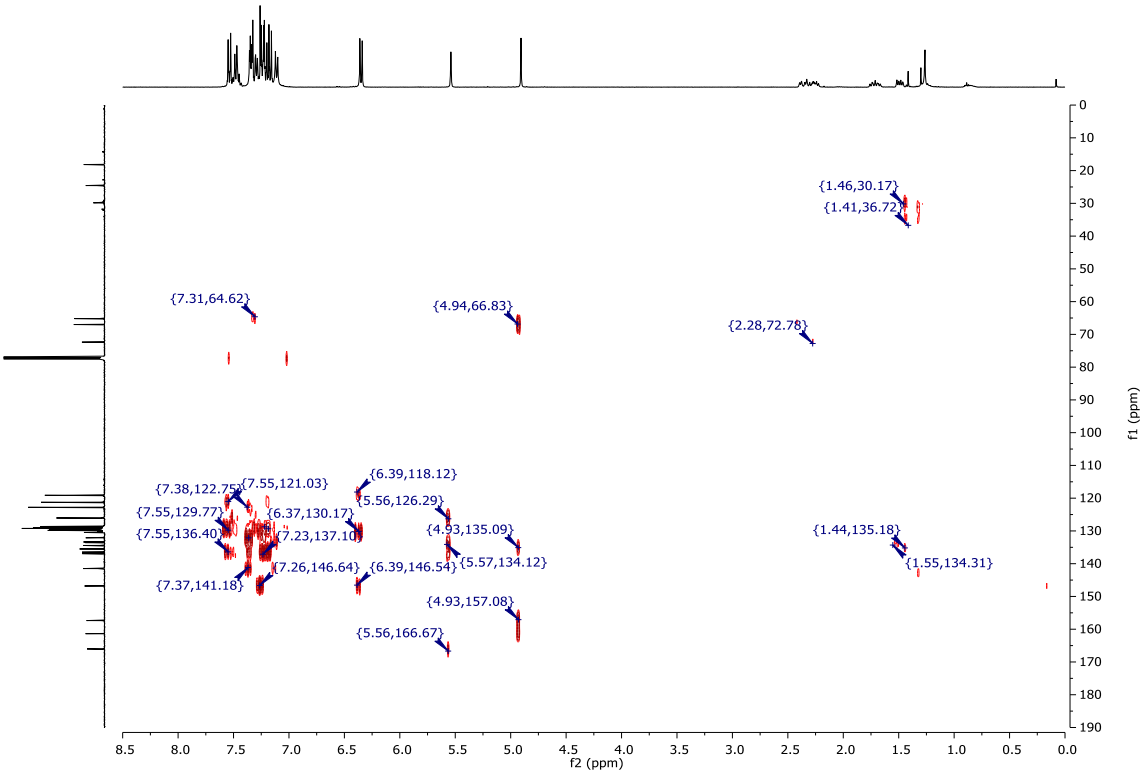
2D-COSY NMR {^{1}H – ^{1}H} (400 MHz, $CDCl_3$)



2D-HSQC NMR {^{1}H – ^{13}C} (^{1}H: 400 MHz, ^{13}C: 101 MHz, $CDCl_3$)



2D-HMBC NMR {^{1}H – ^{13}C} (^{1}H: 400 MHz, ^{13}C: 101 MHz, $CDCl_3$)



VII. Computational methods

Theoretical calculations have been carried out within the DFT framework.[9] Reaction profiles analysis have been carried out at the M06-2X-GD3(PCM)/6-31G* level by using the GAUSSIAN 16[10] suite of programs. Single point energy calculations have been computed at M06-2X(PCM)/6-31+G** from previously optimized structures. This highly parameterized method, well suited for the treatment of nonbonding interactions.[11] Thermal Gibbs corrections were computed at the same level, at the selected temperature, and were not scaled. Solvent effects were estimated by the polarization continuum model[12] (PCM) method within the self-consistent reaction field (SCRF) approach.[13] All SCRF-PCM calculations were performed using chloroform (ε = 4.7113) as model solvent.

All the stationary points were characterized by harmonic vibrational analysis. Local minima showed positive definite Hessians. Fully optimized transition structures showed only one imaginary frequency associated with nuclear motion along the chemical transformation under study. Reaction paths were checked by intrinsic reaction coordinates (IRC) calculations. Activation Gibbs free energies were computing by using stationary points directly connected by IRC calculations.

Representation of the non covalent interactions (NCI plots) were computed using NCIPLOT3[14] program using wavefunctions computed at M06-2X-GD3(PCM)/6-31G* level of optimized structures.

Reaction profiles were analyzed using the distortion/interaction activation strain (ASM) – distortion/interaction model[15] developed by Bickelhaupt – Houk computed at the ZORA–M06-2X-GD3/TZ2P level of theory using the AMS2021[16] suite of programs using previously optimized geometries.

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The energy of the computed stationary points along the reaction coordinate (ΔE (ζ)) was decomposed as:

$$\Delta E\ (\zeta) = \Delta E_{strain}(\zeta) + \Delta E_{int}(\zeta) \quad (1)$$

where $\Delta E_{strain}(\zeta)$ and $\Delta E_{int}(\zeta)$ correspond to the strain and interaction energy, respectively. The strain energy is associated with the energy required to deform the reactants from their equilibrium geometry to the geometry they adopt in that stationary point of the reaction coordinate ζ. This term is dependent of reactants the rigidity and, in general, is positive (destabilizing) giving rise to the occurrence of the reaction barrier. On the other hand, the interaction term $\Delta E_{int}(\zeta)$ depends on the electronic structure of the reagents and on how they approach each other. This latter term can be further analyzed within the Kohn–Sham MO conceptual framework according to the canonical energy decomposition analysis (EDA)[17] as:

$$\Delta E_{int}(\zeta) = \Delta E_{Pauli}(\zeta) + \Delta V_{elstat}\ (\zeta) + \Delta E_{oi}(\zeta) + \Delta E_{disp}(\zeta) \quad (2)$$

ΔV_{elstat} is the classical Coulombic interaction between the unperturbed charge distributions of each of the two reactants. ΔE_{Pauli} is the Pauli repulsions between occupied orbitals of the two fragments and is responsible for steric repulsion. ΔE_{oi} stands for the stabilizing orbital interaction energy, including charge transfer. ΔE_{disp} takes into account the dispersion energy.

Table S5. Energy decomposition analysis terms (in kcal mol^{-1}) computed at the ZORA–M06-2X-GD3/ZV2P level of selected stationary points discussed in the main text.

Structure	$\Delta E_{Pauli}(\zeta)$	$\Delta V_{elstat}\ (\zeta)$	$\Delta E_{oi}(\zeta)$	$\Delta E_{disp}(\zeta)$
AAa$_{homo}$	18.9	–23.6	–12.4	–27.1
AAa$_{hetero}$	19.8	–25.0	–15.1	–25.0
AAa$_{homo\text{-}inin}$	23.1	–18.9	–14.3	–21.4
RCa$_{homo}$	17.2	–25.1	–12.2	–26.1
RCa$_{hetero}$	15.6	–22.0	–11.9	–24.9
RCf$_{homo}$	14.2	–21.1	–12.0	–24.6
RCf$_{hetero}$	13.2	–20.8	–10.2	–22.5
TSa$_{homo}$	110.3	–68.3	–69.0	–28.8
TSa$_{hetero}$	122.5	–70.5	–75.4	–24.4
TSf$_{homo}$	108.5	–69.5	–68.9	–24.7
TSf$_{hetero}$	120.8	–70.4	–73.6	–24.3

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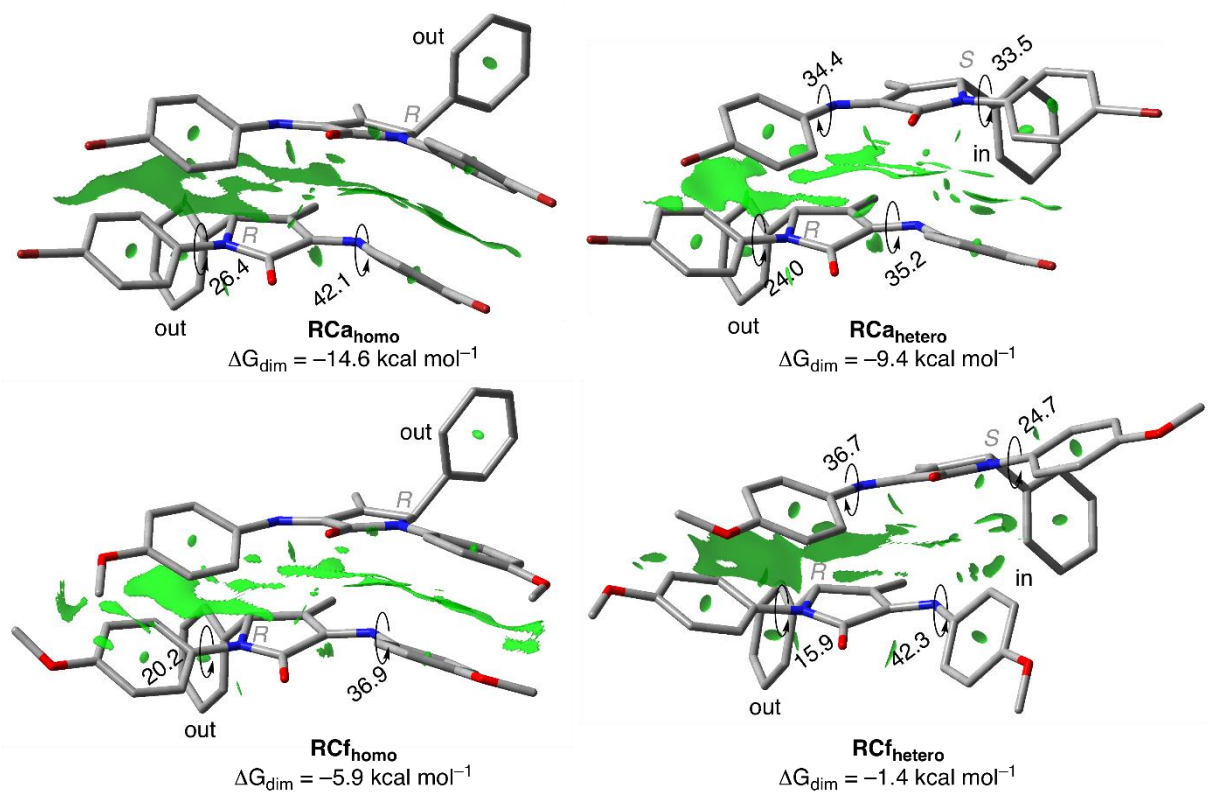

Figure S3. Contour plots of the reduced density gradient isourfaces (RGD, density cutoff = 0.20 au) for the most stable dimeric reactive complexes and Gibbs binding free energies (ΔGb) computed at M06-2X-GD3 (PCM)/6-31+G** // M06-2X-GD3 (PCM)/6-31G* level of theory. Dihedral angles are in deg. The green surfaces indicate attractive non-covalent interactions.

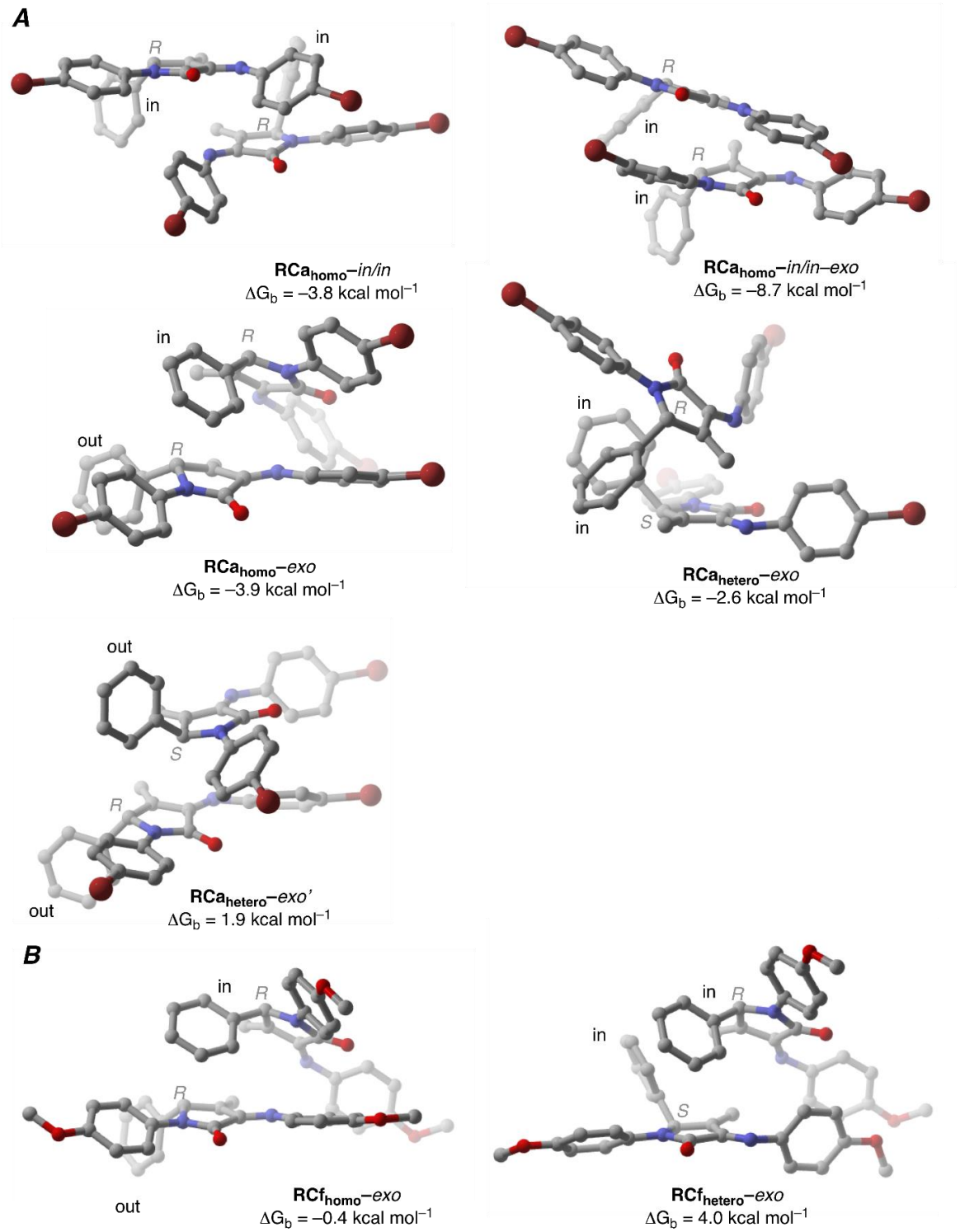

Figure S4. Main geometrical features and Gibbs binding free energies (ΔGb) of all other computed reactive complexes of azadienes (A) **4a** and (B) **4f** computed computed at M06-2X-GD3(PCM)/6-31+G** // M06-2X-GD3(PCM)/6-31G* level of theory. See main manuscript for ΔGb deffinition.

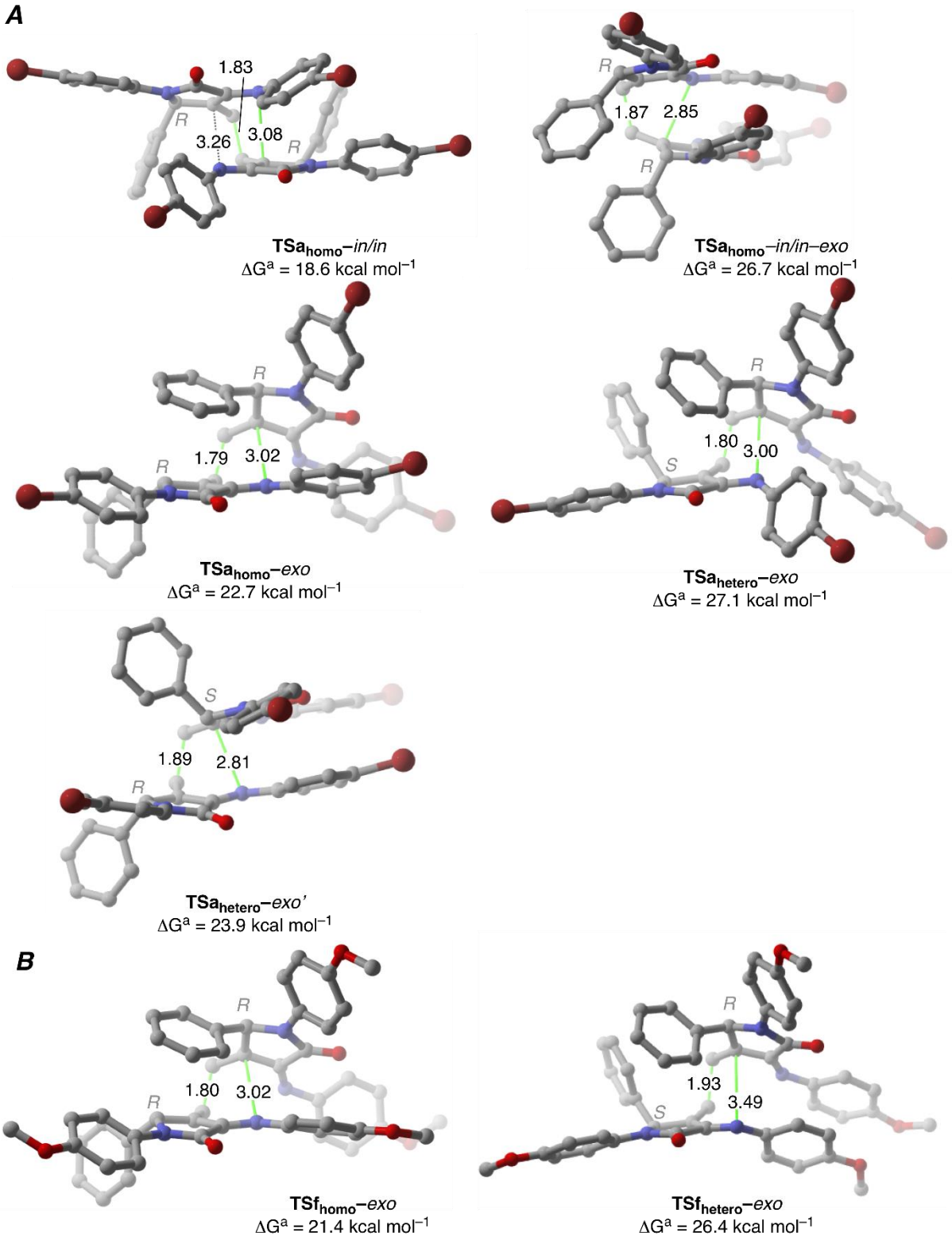

Figure S5. Main geometrical features and Gibbs activation energies computed of all other transition structures associated with the Diels–Alder dimerization of the azadienes **4a** (A) and **4f** (B) computed at M06-2X-GD3(PCM)/6-31+G** // M06-2X-GD3(PCM)/6-31G* level of theory. Distances are in Å.

Evaluation of the reaction profiles associated with less sterically demanding brominated γ–lactams 4g and 4h

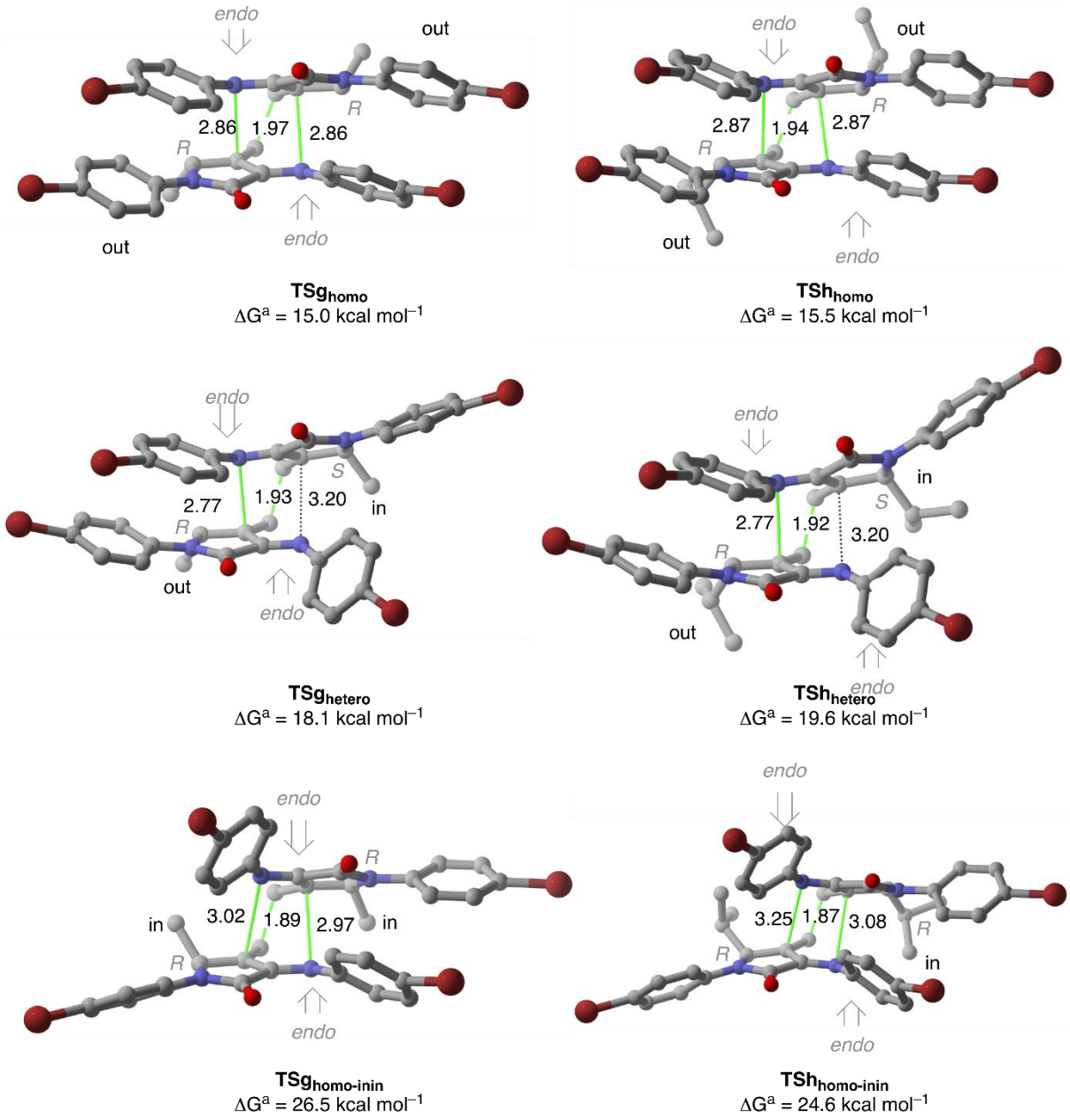

Figure S6. Main geometrical features and Gibbs activation energies computed of transition structures associated with the Diels–Alder dimerization of the γ–lactams **4g** and **4h** computed at M06-2X-GD3 (PCM)/6-31+G** // M06-2X-GD3 (PCM)/6-31G* level of theory. Distances are in Å.

Table S6. Total electronic energies[a] (E, in a.u.), a zero point correction of the energy[b] (ZPE), thermal corrections to Gibbs free energies[b] (TCGFE, in a.u.), and number of imaginary frequencies[c] (NIMAG) of all stationary points discussed in the main text optimized at the M06-2X-GD3(PCM, solvent=chloroform)/6-31G* level of theory.

Structure	E	ZPC[b]	T□□□□[b]	NIMAG[c](□)
3a–R	-6443.069942	0.402704	0.337732	0
3a–S	-6443.061253	0.402655	0.337078	0
AAa$_{homo}$	-12886.194557	0.807344	0.709917	0
AAa$_{hetero}$	-12886.183773	0.815263	0.718809	0
AAa$_{homo\text{-}inin}$	-12886.138760	0.807927	0.707902	
3f–R	-1529.624136	0.489684	0.424507	0
3f–S	-1529.614525	0.489380	0.422872	0
AAf$_{homo}$	-3059.264276	0.980993	0.876095	0
AAf$_{hetero}$	-3059.254862	0.982012	0.882864	0
AAf$_{homo\text{-}inin}$	-3059.243458	0.981007	0.880064	0
4f–R	-6214.028288	0.334777	0.275856	0
4f–S	-6214.028288	0.334780	0.275867	0
RCa$_{homo}$	-12428.109777	0.671122	0.581642	0
RCa$_{hetero}$	-12428.103466	0.671905	0.583647	0
RCa$_{homo}$-in/in	-12428.092348	0.671509	0.580711	0
RCa$_{homo}$–*exo*	-12428.093692	0.671945	0.582731	0
RCa$_{hetero}$–*exo*	-12428.090846	0.671819	0.581854	0
RCa$_{hetero}$–*exo'*	-12428.089542	0.671537	0.579487	0
RCa$_{homo}$-in/in–*exo*	-12428.098943	0.672818	0.586973	0
TSa$_{homo}$	-12428.090668	0.672722	0.588063	1 (-421.6719)
TSa$_{hetero}$	-12428.075359	0.672352	0.585649	1 (-449.0093)
TSa$_{homo}$-in/in	-12428.066963	0.672251	0.584946	1 (-352.7070)
TSa$_{homo}$–*exo*	-12428.058262	0.672037	0.583506	1 (-322.4270)
TSa$_{hetero}$–*exo*	-12428.050903	0.672339	0.585031	1 (-330.2563)
TSa$_{hetero}$–*exo'*	-12428.053441	0.672095	0.581490	1 (-442.8781)
TSa$_{homo}$-in/in–*exo*	-12428.059932	0.673430	0.590582	1 (-439.6471)
5a$_{homo}$	-12428.138629	0.677417	0.592482	0
5a$_{hetero}$	-12428.132423	0.677410	0.593003	0
5a$_{homo}$-in/in	-12428.130832	0.677388	0.588210	0
5a$_{homo}$–*exo*	-12428.143707	0.676505	0.586140	0
5a$_{hetero}$–*exo*	-12428.133161	0.677277	0.589493	0
5a$_{hetero}$–*exo'*	-12428.139966	0.677084	0.587122	0
5a$_{homo}$-in/in–*exo*	-12428.143687	0.677474	0.588714	0
4f–R	-1300.584716	0.421832	0.363005	0
4f–S	-1300.582885	0.421689	0.362583	0
RCf$_{homo}$	-2601.210531	0.845779	0.757677	0
RCf$_{hetero}$	-2601.201051	0.846233	0.756915	0
RCf$_{homo}$–*exo*	-2601.197379	0.845357	0.753068	0
RCf$_{hetero}$–*exo*	-2601.202180	0.846624	0.757936	0
TSf$_{homo}$	-2601.189148	0.847082	0.761785	1 (-442.4727)
TSf$_{hetero}$	-2601.178130	0.846868	0.760705	1 (-470.3287)
TSf$_{homo}$–*exo*	-2601.165158	0.845398	0.755006	1 (-381.6358)

TSf$_{hetero}$–*exo*	-2601.162711	0.846376	0.760478	1 (-578.6753)
5f$_{homo}$	-2601.236495	0.851607	0.767972	0
5f$_{hetero}$	-2601.247537	0.851401	0.762454	0
5f$_{homo}$–*exo*	-2601.249844	0.850269	0.758630	0
5f$_{hetero}$–*exo*	-2601.240642	0.851029	0.762234	0
RCg$_{homo}$	-12044.761501	0.565007	0.487039	0
RCg$_{hetero}$	-12044.751074	0.565247	0.485266	0
RCg$_{homo}$-in/in	-12044.745044	0.565248	0.484640	0
TSg$_{homo}$	-12044.742529	0.566326	0.492035	1 (-437.7381)
TSg$_{hetero}$	-12044.726459	0.566007	0.489557	1 (-444.2235)
TSg$_{homo}$-in/in	-12044.720503	0.565947	0.488322	1 (-433.6041)
5g$_{homo}$	-12044.791901	0.570912	0.496762	0
5g$_{hetero}$	-12044.795174	0.570918	0.493964	0
5g$_{homo}$-in/in	-12044.785020	0.570807	0.491145	0
RCh$_{homo}$	-12201.948434	0.680050	0.595807	0
RCh$_{hetero}$	-12201.935723	0.679861	0.593192:	0
RCh$_{homo}$-in/in	-12201.927983	0.679539	0.592439	0
TSh$_{homo}$	-12201.928761	0.680934	0.599238	1 (-430.0710)
TSh$_{hetero}$	-12201.909324	0.680750	0.598108	1 (-441.2424)
TSh$_{homo}$-in/in	-12201.893755	0.680852	0.597438	1 (-415.9138)
5h$_{homo}$	-12201.977210	0.685641	0.605767	0
5h$_{hetero}$	-12201.973861	0.685686	0.603001	0
5h$_{homo}$-in/in	-12201.973213	0.684748	0.597613	0

[a]Computed at M06-2X-GD3(PCM, solvent=chloroform)/6-31+G** //M06-2X-GD3(PCM, solvent=chloroform)/6-31G* level [b]Computed at 298.15K. [c] If NIMAGE is not zero, imaginary frequency is in cm^{-1}.

Cartesian coordinates (optimized at the B3LYP-D3(PCM, solvent=THF)/6-31G*&LanL2DZ) of all the stationary points analyzed.

3a–R

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.653252	-2.327380	0.646816
2	6	0	1.832322	-1.190617	-0.154498
3	6	0	2.998390	-1.077675	-0.923642
4	6	0	3.964130	-2.076058	-0.898645
5	6	0	3.767172	-3.197955	-0.104960
6	6	0	2.618737	-3.327284	0.664902
7	7	0	0.874462	-0.156293	-0.197828
8	6	0	-0.414300	-0.215393	0.299825
9	6	0	-1.040037	1.112201	-0.011729
10	6	0	-0.138490	1.892187	-0.626962
11	6	0	1.170070	1.155747	-0.771055
12	6	0	-0.305941	3.300324	-1.086459
13	8	0	0.225432	4.188120	-0.088423
14	6	0	1.172142	5.069590	-0.477335
15	8	0	1.510670	5.229593	-1.624610
16	7	0	-2.302376	1.436087	0.441519
17	6	0	-3.446837	0.642151	0.294208
18	6	0	-4.595524	0.982028	1.017685
19	6	0	-5.760629	0.238178	0.885118
20	6	0	-5.774601	-0.860597	0.034070
21	6	0	-4.643731	-1.212101	-0.693570
22	6	0	-3.485718	-0.454011	-0.574101
23	8	0	-0.940972	-1.142515	0.883479
24	6	0	2.318882	1.869069	-0.073267

25	6	0	3.219108	2.627872	-0.818766
26	6	0	4.251095	3.319202	-0.184180
27	6	0	4.393792	3.240488	1.198188
28	6	0	3.492076	2.482213	1.947101
29	6	0	2.454099	1.805591	1.314938
30	35	0	-7.360479	-1.886987	-0.142802
31	35	0	5.082141	-4.563138	-0.069784
32	6	0	1.733697	5.789789	0.715458
33	1	0	0.213772	3.476096	-2.031310
34	1	0	-1.364813	3.541541	-1.214671
35	1	0	1.407645	1.054868	-1.839351
36	1	0	3.112614	2.684927	-1.899854
37	1	0	4.945206	3.909634	-0.773702
38	1	0	5.203462	3.767482	1.693067
39	1	0	3.599278	2.417470	3.025316
40	1	0	1.753211	1.213118	1.897934
41	1	0	3.170960	-0.208372	-1.546708
42	1	0	4.863168	-1.977493	-1.496435
43	1	0	2.474197	-4.204882	1.285116
44	1	0	0.762353	-2.430595	1.248333
45	1	0	-2.613966	-0.715434	-1.163553
46	1	0	-4.669124	-2.064658	-1.363170
47	1	0	-6.648347	0.506612	1.446766
48	1	0	-4.571209	1.830359	1.695569
49	1	0	2.206564	5.056075	1.374945
50	1	0	2.466484	6.524774	0.386533
51	1	0	0.929130	6.276519	1.271781
52	1	0	-2.463360	2.410810	0.659646

3a–S

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.196652	1.345838	1.942645
2	6	0	-1.741998	1.845421	0.759157
3	6	0	-2.714095	2.844317	0.813075
4	6	0	-3.138317	3.343891	2.044107
5	6	0	-2.592775	2.842889	3.223438
6	6	0	-1.624472	1.839861	3.170836
7	6	0	-1.214006	1.375993	-0.584580
8	6	0	0.155318	1.949439	-0.853837
9	6	0	1.027374	0.966812	-1.116102
10	6	0	0.308955	-0.350385	-1.059630
11	7	0	-0.987224	-0.064173	-0.669510
12	6	0	0.376507	3.416035	-0.703204
13	8	0	-0.696315	4.086408	-1.369003
14	6	0	-1.240726	5.226876	-0.879457
15	6	0	-0.635504	5.844222	0.356820
16	7	0	2.348874	1.035875	-1.516074
17	6	0	3.388556	0.286803	-0.952568
18	6	0	3.221749	-0.441195	0.230514
19	6	0	4.278553	-1.171555	0.759601
20	6	0	5.512979	-1.156699	0.121729
21	6	0	5.702762	-0.423137	-1.043819
22	6	0	4.639457	0.290113	-1.580998
23	8	0	0.779653	-1.439534	-1.319705
24	6	0	-2.035483	-0.998270	-0.542186
25	6	0	-3.363435	-0.553921	-0.555771
26	6	0	-4.412160	-1.454126	-0.410151
27	6	0	-4.136125	-2.805271	-0.252534
28	6	0	-2.824820	-3.263772	-0.232563
29	6	0	-1.774123	-2.365120	-0.372115
30	35	0	-5.565177	-4.035761	-0.057023
31	35	0	6.958533	-2.141890	0.856015
32	8	0	-2.193471	5.684423	-1.456340
33	1	0	-1.904745	1.694579	-1.376973
34	1	0	0.375987	3.656158	0.364971
35	1	0	-3.139995	3.233276	-0.109910
36	1	0	-3.896656	4.119758	2.077969
37	1	0	-2.924273	3.227905	4.182488
38	1	0	-1.201545	1.443649	4.088522

39	1	0	-0.440321	0.565496	1.897138
40	1	0	-0.754934	-2.723447	-0.357019
41	1	0	-2.618487	-4.320471	-0.103633
42	1	0	-5.437045	-1.100918	-0.421478
43	1	0	-3.596895	0.497368	-0.674866
44	1	0	2.268532	-0.432033	0.748098
45	1	0	4.144464	-1.738476	1.674173
46	1	0	6.669887	-0.415473	-1.534229
47	1	0	4.775648	0.848758	-2.502432
48	1	0	1.331732	3.736007	-1.129978
49	1	0	-0.848983	5.219528	1.231162
50	1	0	0.447899	5.956819	0.268944
51	1	0	-1.097957	6.819332	0.499331
52	1	0	2.624636	1.867355	-2.021976

AAa$_{homo}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.594160	-1.643119	1.316610
2	6	0	-1.765442	-0.895712	2.483527
3	6	0	-2.852035	-1.179936	3.320929
4	6	0	-3.754205	-2.182291	2.990653
5	6	0	-3.564282	-2.915839	1.824041
6	6	0	-2.485806	-2.655968	0.988601
7	7	0	-0.910934	0.158799	2.832361
8	6	0	0.227993	0.546173	2.149569
9	6	0	0.621876	1.787668	1.808070
10	6	0	2.024155	1.745458	1.242652
11	7	0	2.322052	0.309663	1.241143
12	6	0	1.323720	-0.430622	1.826167
13	6	0	-0.187158	3.042661	1.919807
14	8	0	1.327125	-1.630412	2.033376
15	6	0	3.568300	-0.202155	0.817045
16	6	0	4.183390	0.352876	-0.306711
17	6	0	5.392399	-0.153886	-0.765941
18	6	0	5.979169	-1.219415	-0.096104
19	6	0	5.386639	-1.774537	1.031717
20	6	0	4.182290	-1.257949	1.496019
21	6	0	3.077503	2.488489	2.055004
22	6	0	3.992381	3.331595	1.426675
23	6	0	4.996621	3.957011	2.164412
24	6	0	5.089299	3.740607	3.536560
25	6	0	4.172787	2.900051	4.170370
26	6	0	3.172752	2.275966	3.431727
27	35	0	7.593755	-1.950575	-0.759148
28	35	0	-4.807804	-4.265217	1.355788
29	6	0	0.186786	3.043143	-1.920514
30	6	0	-0.622011	1.787958	-1.808300
31	6	0	-0.227936	0.546467	-2.149622
32	6	0	-1.323448	-0.430476	-1.825951
33	7	0	-2.321826	0.309705	-1.240888
34	6	0	-2.024201	1.745561	-1.242663
35	7	0	0.911019	0.159149	-2.832350
36	6	0	1.765566	-0.895318	-2.483609
37	6	0	1.594543	-1.642629	-1.316561
38	6	0	2.486273	-2.655434	-0.988643
39	6	0	3.564598	-2.915361	-1.824266
40	6	0	3.754276	-2.181912	-2.990973
41	6	0	2.852012	-1.179610	-3.321185
42	6	0	-3.077830	2.488293	-2.054926
43	6	0	-3.992779	3.331257	-1.426505
44	6	0	-4.997256	3.956432	-2.164117
45	6	0	-5.090101	3.739933	-3.536238
46	6	0	-4.173528	2.899515	-4.170142
47	6	0	-3.173258	2.275660	-3.431619
48	6	0	-3.567987	-0.202299	-0.816736
49	6	0	-4.181897	-1.258129	-1.495736
50	6	0	-5.386235	-1.774779	-1.031488
51	6	0	-5.978832	-1.219713	0.096328
52	6	0	-5.392124	-0.154186	0.766223
53	6	0	-4.183123	0.352658	0.307028
54	8	0	-1.326680	-1.630293	-2.033014

55	35	0	-7.593512	-1.950881	0.759153
56	35	0	4.808247	-4.264656	-1.356078
57	1	0	-2.018728	2.138181	-0.216980
58	1	0	-0.471400	3.426307	0.935008
59	1	0	-1.097888	2.859795	2.493503
60	1	0	1.097191	2.860392	-2.494758
61	1	0	0.471622	3.426872	-0.935924
62	1	0	2.018772	2.137888	0.216894
63	1	0	-3.909320	3.511267	-0.357837
64	1	0	-5.705076	4.610411	-1.664809
65	1	0	-5.871975	4.224510	-4.112451
66	1	0	-4.240090	2.729062	-5.239998
67	1	0	-2.460859	1.618182	-3.924654
68	1	0	3.909045	3.511546	0.357989
69	1	0	5.704387	4.611103	1.665175
70	1	0	5.870989	4.225371	4.112864
71	1	0	4.239211	2.729675	5.240248
72	1	0	2.460403	1.618381	3.924690
73	1	0	3.703230	1.160354	-0.850338
74	1	0	5.862317	0.261359	-1.650387
75	1	0	5.858073	-2.607601	1.540877
76	1	0	3.705524	-1.688080	2.367401
77	1	0	-3.705098	-1.688192	-2.367134
78	1	0	-5.857638	-2.607823	-1.540713
79	1	0	-5.862102	0.261032	1.650650
80	1	0	-3.703037	1.160205	0.850626
81	1	0	0.775453	-1.427852	-0.643389
82	1	0	2.353560	-3.206099	-0.063792
83	1	0	4.603339	-2.389701	-3.633339
84	1	0	2.992258	-0.607401	-4.234341
85	1	0	-2.992449	-0.607642	4.234004
86	1	0	-4.603380	-2.390050	3.632879
87	1	0	-2.352896	-3.206709	0.063824
88	1	0	-0.774948	-1.428379	0.643577
89	8	0	0.506505	4.079667	2.626318
90	6	0	1.278529	4.890082	1.876662
91	8	0	1.384300	4.783005	0.676395
92	6	0	1.999574	5.885435	2.736416
93	1	0	2.698063	5.338594	3.378893
94	1	0	2.546974	6.584400	2.106304
95	1	0	1.292096	6.416248	3.377041
96	8	0	-0.507403	4.079999	-2.626719
97	6	0	-1.279349	4.890191	-1.876724
98	8	0	-1.384682	4.782964	-0.676433
99	6	0	-2.000792	5.885569	-2.736122
100	1	0	-1.293480	6.416836	-3.376564
101	1	0	-2.699112	5.338735	-3.378772
102	1	0	-2.548361	6.584179	-2.105761
103	1	0	-1.318842	0.858864	3.438365
104	1	0	1.318718	0.859070	-3.438631

AAa$_{hetero}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.816442	-0.172509	-1.828067
2	6	0	-3.519707	-0.698992	-1.816899
3	6	0	-3.337069	-2.059936	-1.533825
4	6	0	-4.428720	-2.865809	-1.242533
5	6	0	-5.704627	-2.317540	-1.215113
6	6	0	-5.907570	-0.978541	-1.519311
7	7	0	-2.411140	0.149202	-2.025374
8	6	0	-1.131584	-0.272877	-2.326088
9	6	0	-0.273719	0.964026	-2.350054
10	6	0	-1.071652	2.038286	-2.225474
11	6	0	-2.510306	1.605218	-2.050937
12	6	0	-0.727388	3.488882	-2.232773
13	8	0	-1.445349	4.094223	-3.315462
14	6	0	-1.653224	5.435453	-3.336233
15	6	0	-1.127195	6.253940	-2.184393
16	7	0	1.090341	0.908348	-2.578347
17	6	0	1.902102	-0.193479	-2.259828
18	6	0	1.652509	-0.965306	-1.119619

19	6	0	2.436094	-2.075656	-0.833552
20	6	0	3.501983	-2.393157	-1.670020
21	6	0	3.801241	-1.601572	-2.772374
22	6	0	2.999494	-0.504703	-3.067554
23	8	0	-0.770744	-1.406873	-2.568160
24	6	0	-3.139460	2.217604	-0.812647
25	6	0	-3.845933	3.414953	-0.937384
26	6	0	-4.436428	4.003638	0.178200
27	6	0	-4.327013	3.392366	1.424201
28	6	0	-3.609581	2.202969	1.553308
29	6	0	-3.012259	1.615607	0.440301
30	35	0	4.566217	-3.917252	-1.308738
31	35	0	-7.171344	-3.412455	-0.730176
32	8	0	-2.260612	5.895452	-4.268786
33	6	0	0.160236	2.936119	1.037160
34	8	0	-0.522449	3.428640	2.196270
35	6	0	-1.319486	4.490503	1.951872
36	6	0	-1.988421	4.979786	3.203067
37	6	0	1.002038	1.770295	1.415511
38	6	0	0.653161	0.705261	2.147846
39	6	0	1.803574	-0.251234	2.198587
40	7	0	2.833676	0.352714	1.495520
41	6	0	2.417741	1.626410	0.923338
42	7	0	-0.515193	0.520214	2.877056
43	6	0	-1.394955	-0.557894	2.698263
44	6	0	-2.579865	-0.565529	3.446891
45	6	0	-3.543593	-1.543105	3.245060
46	6	0	-3.311773	-2.548675	2.313029
47	6	0	-2.119960	-2.589146	1.599936
48	6	0	-1.166019	-1.591742	1.782974
49	35	0	-4.643857	-3.861795	2.009996
50	6	0	3.289156	2.799917	1.330429
51	6	0	3.598894	3.788855	0.397438
52	6	0	4.343643	4.904582	0.775577
53	6	0	4.786945	5.028979	2.089309
54	6	0	4.481979	4.038493	3.023450
55	6	0	3.731053	2.929661	2.647577
56	6	0	4.055582	-0.250688	1.133613
57	6	0	4.803277	0.284981	0.079143
58	6	0	5.962363	-0.347524	-0.354781
59	6	0	6.381967	-1.509822	0.274014
60	6	0	5.676791	-2.029339	1.352174
61	6	0	4.519153	-1.399993	1.789457
62	8	0	1.810850	-1.345569	2.730354
63	35	0	7.893094	-2.436667	-0.386858
64	8	0	-1.421030	4.979153	0.851572
65	1	0	-3.091907	1.916808	-2.930791
66	1	0	0.762148	3.739074	0.598961
67	1	0	-0.592090	2.625565	0.304066
68	1	0	-1.032849	3.947422	-1.284901
69	1	0	2.401746	1.549195	-0.175728
70	1	0	-3.951326	3.875053	-1.918074
71	1	0	-4.991361	4.929978	0.069918
72	1	0	-4.805529	3.834713	2.292736
73	1	0	-3.544271	1.709016	2.518323
74	1	0	-2.480428	0.669301	0.536682
75	1	0	3.262201	3.680705	-0.632407
76	1	0	4.582641	5.668688	0.042678
77	1	0	5.372703	5.893296	2.385515
78	1	0	4.830277	4.131335	4.047262
79	1	0	3.491270	2.155622	3.372292
80	1	0	4.480906	1.180593	-0.437491
81	1	0	6.520241	0.054688	-1.193213
82	1	0	6.017162	-2.936722	1.838668
83	1	0	3.959191	-1.815523	2.614402
84	1	0	-2.345344	-2.487151	-1.542323
85	1	0	-4.279494	-3.913759	-1.009436
86	1	0	-6.907120	-0.558814	-1.508573
87	1	0	-4.988333	0.873946	-2.052424
88	1	0	0.827465	-0.697368	-0.462035
89	1	0	2.235911	-2.672916	0.050702
90	1	0	4.645625	-1.849042	-3.406477
91	1	0	3.209440	0.095324	-3.948660
92	1	0	-0.242069	-1.632816	1.217478

93	1	0	-1.936528	-3.388036	0.889679
94	1	0	-4.468139	-1.525357	3.811215
95	1	0	-2.746505	0.209803	4.190013
96	1	0	0.351152	3.635870	-2.364322
97	1	0	-0.066344	6.058570	-2.002189
98	1	0	-1.270624	7.305229	-2.428510
99	1	0	-1.667003	6.013480	-1.262326
100	1	0	-2.410416	4.141659	3.761426
101	1	0	-1.242705	5.468030	3.837235
102	1	0	-2.768214	5.692558	2.939041
103	1	0	-0.974694	1.396355	3.105121
104	1	0	1.458085	1.545879	-3.273261

AAa$_{\text{homo-inin}}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.728269	1.062243	-1.285874
2	6	0	-4.622058	0.221975	-1.459788
3	6	0	-4.815431	-1.166115	-1.488991
4	6	0	-6.093751	-1.694760	-1.352200
5	6	0	-7.179327	-0.845920	-1.178914
6	6	0	-7.004246	0.531190	-1.143571
7	7	0	-3.332132	0.785308	-1.571488
8	6	0	-3.041514	2.162422	-1.169290
9	6	0	-1.569737	2.297951	-1.508425
10	6	0	-1.110956	1.153481	-2.040577
11	6	0	-2.226375	0.157887	-2.108963
12	7	0	0.096811	0.914720	-2.662837
13	6	0	0.873179	-0.245493	-2.512630
14	6	0	0.629062	-1.182992	-1.505251
15	6	0	1.464477	-2.282509	-1.348754
16	6	0	2.573639	-2.418514	-2.175960
17	6	0	2.834303	-1.497351	-3.183633
18	6	0	1.970218	-0.424060	-3.363268
19	35	0	3.774887	-3.858634	-1.896744
20	6	0	-0.821206	3.594237	-1.389535
21	8	0	-1.791599	4.596014	-1.105666
22	6	0	-1.451811	5.867957	-0.774500
23	6	0	0.010749	6.220598	-0.734908
24	6	0	-3.392134	2.404083	0.294841
25	6	0	-3.939135	3.619098	0.710827
26	6	0	-4.295923	3.805354	2.045310
27	6	0	-4.100756	2.786933	2.976455
28	6	0	-3.560970	1.568837	2.565219
29	6	0	-3.222587	1.379861	1.227997
30	8	0	-2.168411	-0.965081	-2.571315
31	35	0	-8.917778	-1.574523	-0.986308
32	8	0	-2.345645	6.629006	-0.510660
33	6	0	3.044912	4.611123	-0.462400
34	6	0	2.944888	3.783622	0.655344
35	6	0	2.787322	2.405007	0.496407
36	6	0	2.749246	1.861170	-0.788117
37	6	0	2.863474	2.688847	-1.902720
38	6	0	3.000492	4.067778	-1.744822
39	6	0	2.619930	1.502208	1.713671
40	6	0	1.166561	1.206571	1.982441
41	6	0	0.916020	-0.103402	1.843009
42	6	0	2.205249	-0.819529	1.586005
43	7	0	3.172382	0.165004	1.509869
44	7	0	-0.341503	-0.675618	1.809258
45	6	0	-0.676329	-2.039233	1.843415
46	6	0	-0.061412	-2.924902	2.734041
47	6	0	-0.447991	-4.257117	2.768474
48	6	0	-1.470528	-4.700753	1.933840
49	6	0	-2.104985	-3.831756	1.056853
50	6	0	-1.698158	-2.502701	1.008778
51	35	0	-2.007520	-6.517664	2.000640
52	6	0	0.158894	2.275588	2.233140
53	8	0	0.865677	3.404241	2.743574
54	6	0	0.349634	4.652078	2.653422
55	6	0	-1.121486	4.777237	2.366473
56	6	0	4.506329	-0.045311	1.097545

57	6	0	5.485518	0.899971	1.415834
58	6	0	6.790331	0.739306	0.962229
59	6	0	7.113393	-0.368154	0.188168
60	6	0	6.149499	-1.313344	-0.142228
61	6	0	4.847364	-1.152055	0.311651
62	8	0	2.381598	-2.017885	1.477333
63	35	0	8.890824	-0.584345	-0.435707
64	8	0	1.092927	5.584685	2.829166
65	1	0	-3.612380	2.863647	-1.791853
66	1	0	-0.602750	1.933658	2.946900
67	1	0	-0.305082	3.829208	-2.330413
68	1	0	3.077771	1.979868	2.588438
69	1	0	-4.073587	4.424860	-0.005400
70	1	0	-4.725625	4.752377	2.356542
71	1	0	-4.381523	2.935196	4.014297
72	1	0	-3.427544	0.757810	3.274852
73	1	0	-2.891642	0.401802	0.885102
74	1	0	2.979695	4.214331	1.651929
75	1	0	3.169393	5.681467	-0.326674
76	1	0	3.096287	4.710506	-2.614674
77	1	0	2.879776	2.251068	-2.898104
78	1	0	2.659014	0.784894	-0.915924
79	1	0	5.237922	1.771036	2.013060
80	1	0	7.548032	1.473983	1.210062
81	1	0	6.396255	-2.168640	-0.762675
82	1	0	4.099539	-1.887282	0.051774
83	1	0	-3.975118	-1.830012	-1.636222
84	1	0	-6.239590	-2.768891	-1.377447
85	1	0	-7.855010	1.189051	-1.007403
86	1	0	-5.608010	2.138894	-1.254362
87	1	0	-0.205938	-1.052457	-0.826579
88	1	0	1.277159	-2.996462	-0.554534
89	1	0	3.699426	-1.619156	-3.825657
90	1	0	2.149064	0.284702	-4.166752
91	1	0	-2.172927	-1.827021	0.299423
92	1	0	-2.897751	-4.185407	0.407220
93	1	0	0.033873	-4.947050	3.452047
94	1	0	0.724489	-2.569861	3.390654
95	1	0	-0.361533	2.537273	1.300951
96	1	0	-0.049864	3.550379	-0.603830
97	1	0	-1.392847	4.330996	1.404293
98	1	0	-1.700536	4.244949	3.127494
99	1	0	-1.393526	5.832303	2.360819
100	1	0	0.539597	5.876138	-1.627220
101	1	0	0.097149	7.301956	-0.642400
102	1	0	0.491359	5.756276	0.134104
103	1	0	-1.054335	-0.071605	1.420719
104	1	0	0.625939	1.740427	-2.917918

3f-R

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.140224	-1.418750	1.533960
2	6	0	-2.210098	-1.157485	0.163808
3	6	0	-3.442070	-1.229225	-0.484028
4	6	0	-4.596076	-1.556529	0.227548
5	6	0	-4.521867	-1.812442	1.593764
6	6	0	-3.289514	-1.745099	2.246402
7	6	0	-0.956711	-0.740836	-0.595774
8	7	0	-0.475748	0.556555	-0.106013
9	6	0	0.773396	0.465962	0.457952
10	6	0	1.226507	-0.947666	0.224417
11	6	0	0.244838	-1.633616	-0.387838
12	6	0	-1.306392	1.702111	-0.059690
13	6	0	-1.274367	2.579382	1.032655
14	6	0	-2.108938	3.683555	1.058964
15	6	0	-3.005660	3.927526	0.012396
16	6	0	-3.050399	3.050773	-1.071353
17	6	0	-2.195652	1.949931	-1.102158
18	8	0	-3.786336	5.032506	0.142531
19	8	0	1.387693	1.347292	1.030467
20	7	0	2.441733	-1.382842	0.711237

21	6	0	3.664360	-0.714325	0.467119
22	6	0	4.783598	-1.065150	1.231669
23	6	0	6.005940	-0.453409	1.013031
24	6	0	6.133853	0.542775	0.038714
25	6	0	5.022959	0.899625	-0.724598
26	6	0	3.801017	0.259605	-0.517893
27	6	0	0.304236	-3.036613	-0.895453
28	8	0	-0.752629	-3.845945	-0.358408
29	6	0	-1.878043	-3.923657	-1.097239
30	6	0	-2.940912	-4.688790	-0.364000
31	8	0	7.372398	1.095387	-0.090909
32	8	0	-1.994257	-3.415221	-2.187845
33	1	0	0.235544	-3.051117	-1.986501
34	1	0	1.232985	-3.523197	-0.593306
35	1	0	-1.189780	-0.690217	-1.667682
36	1	0	-3.496388	-1.041470	-1.553241
37	1	0	-5.550139	-1.609462	-0.287486
38	1	0	-5.418728	-2.065674	2.150477
39	1	0	-3.225607	-1.945865	3.311265
40	1	0	-1.179846	-1.364437	2.041597
41	1	0	-2.227537	1.283934	-1.958682
42	1	0	-3.733017	3.210711	-1.897120
43	1	0	-2.092044	4.372852	1.896698
44	1	0	-0.588200	2.394375	1.849027
45	1	0	2.952160	0.526200	-1.139506
46	1	0	5.091938	1.660629	-1.492743
47	1	0	6.878617	-0.722697	1.598828
48	1	0	4.684022	-1.820241	2.006443
49	1	0	-3.213147	-4.123726	0.533706
50	1	0	-3.813108	-4.808953	-1.004546
51	1	0	-2.557524	-5.662149	-0.049688
52	1	0	2.526515	-2.383970	0.836547
53	6	0	-4.704737	5.304640	-0.897669
54	1	0	-5.227686	6.216026	-0.609768
55	1	0	-4.188096	5.465647	-1.850837
56	1	0	-5.428009	4.488947	-1.011434
57	6	0	7.526907	2.112829	-1.059341
58	1	0	8.567828	2.430212	-1.003644
59	1	0	7.313706	1.738257	-2.067460
60	1	0	6.872983	2.966508	-0.846392

3f-S

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.618228	-2.153488	-0.382467
2	6	0	-2.535738	-0.789001	-0.667012
3	6	0	-3.720864	-0.075323	-0.895333
4	6	0	-4.948918	-0.713779	-0.846448
5	6	0	-5.027728	-2.082360	-0.575089
6	6	0	-3.853316	-2.798066	-0.343644
7	7	0	-1.291197	-0.117311	-0.696691
8	6	0	-1.188235	1.334468	-0.630033
9	6	0	0.297809	1.574943	-0.738913
10	6	0	0.950457	0.408966	-0.878117
11	6	0	-0.062437	-0.702020	-0.922857
12	6	0	-1.759596	1.925475	0.647220
13	6	0	-1.485585	1.327961	1.878888
14	6	0	-1.960953	1.899810	3.053568
15	6	0	-2.706003	3.078992	3.007090
16	6	0	-2.976847	3.680082	1.781552
17	6	0	-2.505655	3.101602	0.603399
18	6	0	0.811823	2.973776	-0.651807
19	8	0	2.178088	2.975976	-1.060956
20	6	0	2.950937	4.082896	-0.935762
21	8	0	4.096658	4.010548	-1.295385
22	7	0	2.283446	0.141827	-1.110330
23	6	0	2.984022	-0.889240	-0.437400
24	6	0	2.516610	-1.467017	0.748917
25	6	0	3.242930	-2.464628	1.377607
26	6	0	4.468287	-2.889499	0.853745
27	6	0	4.954174	-2.301803	-0.314243
28	6	0	4.204111	-1.316416	-0.954875

29	8	0	0.163273	-1.878826	-1.130934
30	8	0	5.109472	-3.868423	1.552351
31	8	0	-6.278006	-2.617642	-0.555669
32	6	0	2.318759	5.317951	-0.347660
33	1	0	-1.701093	1.785005	-1.493135
34	1	0	0.223125	3.637502	-1.299986
35	1	0	-2.725587	3.563676	-0.356902
36	1	0	-3.560600	4.594132	1.738320
37	1	0	-3.076947	3.523643	3.925081
38	1	0	-1.751185	1.426447	4.007570
39	1	0	-0.906062	0.408286	1.909128
40	1	0	-1.715395	-2.719637	-0.200634
41	1	0	-3.878147	-3.858972	-0.124871
42	1	0	-5.867412	-0.163106	-1.019850
43	1	0	-3.694427	0.987939	-1.106241
44	1	0	1.583222	-1.126545	1.186931
45	1	0	2.884239	-2.922440	2.293733
46	1	0	5.901471	-2.605252	-0.743851
47	1	0	4.571241	-0.874715	-1.876787
48	1	0	0.717048	3.343643	0.377318
49	1	0	1.409444	5.595601	-0.886944
50	1	0	2.050785	5.147960	0.699292
51	1	0	3.042596	6.128526	-0.405819
52	1	0	2.833890	0.969448	-1.309361
53	6	0	6.345139	-4.322918	1.039748
54	1	0	6.691342	-5.098226	1.722736
55	1	0	6.227121	-4.747451	0.035887
56	1	0	7.083279	-3.512994	1.003767
57	6	0	-6.385969	-4.000656	-0.281119
58	1	0	-7.449821	-4.233836	-0.311689
59	1	0	-5.859616	-4.597078	-1.035174
60	1	0	-5.988065	-4.240469	0.711646

AAf_{homo}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.571656	-1.496256	0.466825
2	6	0	-3.833584	-1.326733	-0.702877
3	6	0	-3.938978	-2.287456	-1.718373
4	6	0	-4.716900	-3.416768	-1.522787
5	6	0	-5.416127	-3.608613	-0.326863
6	6	0	-5.364281	-2.624625	0.658026
7	7	0	-2.999885	-0.190496	-0.841422
8	6	0	-1.898190	-0.101895	-1.654127
9	6	0	-1.304112	1.259777	-1.406005
10	6	0	-2.102887	1.926485	-0.549351
11	6	0	-3.234492	1.037572	-0.096812
12	6	0	-1.995359	3.338395	-0.077078
13	8	0	-2.925444	4.154275	-0.809736
14	6	0	-3.796402	4.898434	-0.096505
15	6	0	-4.779753	5.570106	-1.012542
16	7	0	-0.227715	1.771766	-2.102511
17	6	0	1.014976	1.182639	-2.412446
18	6	0	1.309983	-0.180625	-2.255085
19	6	0	2.549976	-0.674678	-2.626838
20	6	0	3.538045	0.166912	-3.150256
21	6	0	3.271832	1.530765	-3.266073
22	6	0	2.017965	2.023760	-2.900006
23	8	0	-1.505691	-0.945542	-2.442256
24	6	0	-4.615522	1.619568	-0.349940
25	6	0	-5.333238	2.194896	0.695908
26	6	0	-6.588553	2.757873	0.463619
27	6	0	-7.136741	2.730899	-0.815167
28	6	0	-6.419735	2.154358	-1.865629
29	6	0	-5.161930	1.607893	-1.635378
30	8	0	4.708406	-0.429271	-3.505985
31	8	0	-6.103607	-4.776711	-0.215925
32	8	0	-3.776618	4.989456	1.107264
33	8	0	1.029557	4.808065	1.023580
34	6	0	1.488326	4.228295	1.981826
35	6	0	2.138982	4.874113	3.172735
36	8	0	1.482939	2.891079	2.106390

37	6	0	0.997553	2.156160	0.968191
38	6	0	1.609461	0.807205	0.949917
39	6	0	1.055658	-0.363561	1.312298
40	6	0	2.082637	-1.451299	1.142341
41	7	0	3.214686	-0.835334	0.653309
42	6	0	3.025339	0.599928	0.485625
43	7	0	-0.169997	-0.586731	1.889325
44	6	0	-0.974201	-1.738855	1.755746
45	6	0	-0.923956	-2.557217	0.630358
46	6	0	-1.714198	-3.702326	0.545569
47	6	0	-2.595490	-4.018430	1.578915
48	6	0	-2.672718	-3.181352	2.695937
49	6	0	-1.867008	-2.058342	2.786030
50	8	0	-3.425837	-5.100929	1.584687
51	6	0	4.014353	1.457285	1.253407
52	6	0	4.448332	2.656172	0.688517
53	6	0	5.286567	3.509054	1.404764
54	6	0	5.702146	3.157951	2.687517
55	6	0	5.272957	1.955679	3.251257
56	6	0	4.428351	1.110220	2.538732
57	6	0	4.429164	-1.474785	0.308127
58	6	0	5.361535	-0.793432	-0.488795
59	6	0	6.564288	-1.385321	-0.832428
60	6	0	6.870778	-2.676861	-0.395843
61	6	0	5.950965	-3.360620	0.397762
62	6	0	4.742457	-2.761605	0.751988
63	8	0	1.945109	-2.631046	1.410506
64	8	0	8.074997	-3.173022	-0.790418
65	1	0	-3.121449	0.852205	0.982932
66	1	0	1.255178	2.710344	0.058597
67	1	0	-0.091565	2.083121	1.036768
68	1	0	-0.995332	3.753589	-0.235515
69	1	0	-2.227693	3.416306	0.989357
70	1	0	3.087412	0.862262	-0.579743
71	1	0	-4.909394	2.209738	1.697483
72	1	0	-7.137726	3.206595	1.285289
73	1	0	-8.118687	3.156858	-0.996081
74	1	0	-6.843227	2.129954	-2.864885
75	1	0	-4.604055	1.154652	-2.451069
76	1	0	4.128876	2.918059	-0.319372
77	1	0	5.620575	4.440484	0.957974
78	1	0	6.362198	3.815258	3.245046
79	1	0	5.598297	1.677323	4.248875
80	1	0	4.089530	0.174365	2.976349
81	1	0	5.149373	0.207635	-0.848315
82	1	0	7.285258	-0.857367	-1.448363
83	1	0	6.157128	-4.361817	0.757171
84	1	0	4.040107	-3.303377	1.368701
85	1	0	-3.390820	-2.160392	-2.641158
86	1	0	-4.791047	-4.177183	-2.294193
87	1	0	-5.898881	-2.737602	1.593612
88	1	0	-4.519571	-0.761245	1.262452
89	1	0	0.564661	-0.858231	-1.864910
90	1	0	2.780832	-1.728467	-2.504750
91	1	0	4.015425	2.220737	-3.647842
92	1	0	1.819527	3.087290	-3.010375
93	1	0	-1.910018	-1.428346	3.670627
94	1	0	-3.369722	-3.434285	3.488725
95	1	0	-1.651341	-4.317220	-0.344310
96	1	0	-0.254604	-2.311205	-0.188284
97	1	0	3.164595	4.504185	3.261390
98	1	0	2.133263	5.955996	3.051517
99	1	0	1.602039	4.594217	4.082473
100	1	0	-5.333838	4.800101	-1.557029
101	1	0	-5.463955	6.182515	-0.427472
102	1	0	-4.248310	6.185411	-1.742581
103	1	0	-0.595667	0.204361	2.353409
104	1	0	-0.201616	2.784473	-2.117491
105	6	0	8.406109	-4.480044	-0.365295
106	1	0	9.390287	-4.694444	-0.780897
107	1	0	8.450272	-4.542909	0.728190
108	1	0	7.683641	-5.214270	-0.740008
109	6	0	5.780620	0.416186	-3.863998
110	1	0	6.634116	-0.235838	-4.048710

111	1	0	5.555841	0.987010	-4.772533
112	1	0	6.022270	1.114775	-3.051572
113	6	0	-3.277763	-6.036166	0.533479
114	1	0	-3.996297	-6.831641	0.732555
115	1	0	-3.502501	-5.582068	-0.437573
116	1	0	-2.262017	-6.448713	0.519089
117	6	0	-6.687891	-5.062428	1.041673
118	1	0	-7.121913	-6.058432	0.953691
119	1	0	-5.926105	-5.055739	1.828984
120	1	0	-7.479598	-4.344013	1.284447

AAf_{hetero}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.167638	-1.800228	1.163622
2	6	0	3.447530	-0.842034	0.452473
3	6	0	3.878830	-0.472077	-0.825191
4	6	0	5.010427	-1.049941	-1.376265
5	6	0	5.723874	-2.019885	-0.666918
6	6	0	5.295397	-2.397875	0.605105
7	7	0	2.304515	-0.221521	1.013222
8	6	0	1.450986	-0.812195	1.914131
9	6	0	0.500133	0.265488	2.348583
10	6	0	0.841545	1.425765	1.763569
11	6	0	2.013064	1.203802	0.829814
12	6	0	0.127199	2.727919	1.905355
13	8	0	1.024884	3.803906	2.218001
14	6	0	1.432281	4.571021	1.196830
15	8	0	1.049298	4.422628	0.056312
16	7	0	-0.470181	-0.021198	3.291076
17	6	0	-1.378059	-1.092474	3.070042
18	6	0	-2.065550	-1.647209	4.151563
19	6	0	-2.956184	-2.689465	3.952066
20	6	0	-3.160072	-3.216492	2.671616
21	6	0	-2.479811	-2.666888	1.583365
22	6	0	-1.607647	-1.600527	1.794271
23	8	0	1.466155	-1.966545	2.300007
24	6	0	3.242878	2.056972	1.089710
25	6	0	3.781166	2.847925	0.076921
26	6	0	4.936984	3.595871	0.301188
27	6	0	5.562068	3.551215	1.543532
28	6	0	5.023503	2.763184	2.563861
29	6	0	3.869247	2.019745	2.337573
30	8	0	-4.034513	-4.255016	2.590787
31	8	0	6.813982	-2.543258	-1.299682
32	6	0	2.413574	5.606799	1.662095
33	6	0	-0.199645	2.258406	-2.129128
34	8	0	-0.846939	3.025884	-3.156176
35	6	0	-0.244471	4.121013	-3.682752
36	8	0	-0.870114	4.786681	-4.466500
37	6	0	-1.050418	1.066323	-1.861793
38	6	0	-0.738283	-0.231276	-2.032129
39	6	0	-1.940731	-1.067665	-1.701068
40	7	0	-2.947590	-0.186741	-1.358319
41	6	0	-2.503125	1.200755	-1.471450
42	6	0	-4.323716	-0.512109	-1.233277
43	6	0	-5.274419	0.509268	-1.165666
44	6	0	-6.634047	0.227290	-1.044741
45	6	0	-7.070253	-1.094811	-0.993517
46	6	0	-6.124943	-2.121217	-1.071115
47	6	0	-4.772671	-1.843120	-1.186193
48	8	0	-8.368574	-1.478959	-0.876976
49	8	0	-2.007119	-2.282818	-1.762133
50	7	0	0.375612	-0.775840	-2.626440
51	6	0	1.110891	-1.899584	-2.191263
52	6	0	0.938506	-2.475894	-0.929761
53	6	0	1.765684	-3.504775	-0.514532
54	6	0	2.789036	-3.974277	-1.343737
55	6	0	2.939796	-3.432165	-2.619723
56	6	0	2.095928	-2.405233	-3.035972
57	6	0	-2.720523	2.034231	-0.218468
58	6	0	-2.703322	3.427262	-0.328792

59	6	0	-2.920885	4.225091	0.793506
60	6	0	-3.178456	3.636235	2.029893
61	6	0	-3.200926	2.246714	2.140746
62	6	0	-2.964488	1.447552	1.024212
63	8	0	3.586674	-4.948562	-0.821731
64	6	0	1.174459	4.413886	-3.265495
65	1	0	-3.041676	1.679925	-2.302669
66	1	0	-0.431437	2.979856	1.000352
67	1	0	-0.577520	2.690517	2.734812
68	1	0	-0.084048	2.882527	-1.234039
69	1	0	1.672205	1.386363	-0.201662
70	1	0	-2.530733	3.886496	-1.300111
71	1	0	-2.905488	5.305820	0.695571
72	1	0	-3.367048	4.257037	2.900239
73	1	0	-3.416584	1.776459	3.096573
74	1	0	-3.011774	0.366807	1.111078
75	1	0	3.286442	2.884129	-0.890799
76	1	0	5.344759	4.209305	-0.494119
77	1	0	6.463749	4.129115	1.721528
78	1	0	5.506990	2.726525	3.535537
79	1	0	3.447847	1.400405	3.129000
80	1	0	3.318962	0.264509	-1.395601
81	1	0	5.353009	-0.773477	-2.368061
82	1	0	5.827660	-3.149244	1.176350
83	1	0	3.835894	-2.096890	2.150238
84	1	0	-4.064123	-2.654151	-1.266631
85	1	0	-6.473680	-3.148986	-1.043742
86	1	0	-7.332596	1.053695	-0.994135
87	1	0	-4.975585	1.549941	-1.201451
88	1	0	0.174993	-2.108177	-0.254496
89	1	0	1.665668	-3.913836	0.484848
90	1	0	3.715071	-3.781185	-3.291536
91	1	0	2.223709	-1.975106	-4.026114
92	1	0	-1.120140	-1.129651	0.943686
93	1	0	-2.616119	-3.035577	0.572879
94	1	0	-3.499399	-3.126899	4.783702
95	1	0	-1.887968	-1.260901	5.150693
96	1	0	0.798880	1.942353	-2.454770
97	1	0	1.251437	4.537667	-2.180916
98	1	0	1.836006	3.593917	-3.562911
99	1	0	1.490072	5.327076	-3.767415
100	1	0	1.941967	6.253976	2.407692
101	1	0	3.259302	5.099222	2.136486
102	1	0	2.756547	6.196347	0.812064
103	1	0	-0.883189	0.786996	3.742985
104	1	0	0.893862	-0.146163	-3.225039
105	6	0	-4.299130	-4.773437	1.300968
106	1	0	-5.014915	-5.583281	1.438308
107	1	0	-4.736488	-4.003968	0.654396
108	1	0	-3.388772	-5.166336	0.834338
109	6	0	-9.341691	-0.455203	-0.808076
110	1	0	-10.304337	-0.957392	-0.720976
111	1	0	-9.182770	0.184451	0.067754
112	1	0	-9.332344	0.162163	-1.713444
113	6	0	7.653260	-3.392690	-0.540909
114	1	0	8.494946	-3.642932	-1.186436
115	1	0	8.017055	-2.883900	0.358908
116	1	0	7.133962	-4.312712	-0.248986
117	6	0	4.694315	-5.349338	-1.600972
118	1	0	5.248157	-6.068955	-0.997013
119	1	0	4.374575	-5.832675	-2.532340
120	1	0	5.338259	-4.493517	-1.842897

$AAf_{homo\text{-}inin}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.207345	0.748647	0.183143
2	6	0	-4.702059	-0.305245	0.942179
3	6	0	-5.518201	-1.408202	1.212086
4	6	0	-6.819643	-1.445927	0.738493
5	6	0	-7.333258	-0.378680	-0.005813
6	6	0	-6.519769	0.721907	-0.281707

7	7	0	-3.355986	-0.290339	1.381553
8	6	0	-2.534732	-1.489370	1.458122
9	6	0	-1.199773	-0.929296	1.895739
10	6	0	-1.277525	0.398625	2.087412
11	6	0	-2.691248	0.830812	1.810190
12	6	0	-2.479168	-2.261813	0.148937
13	6	0	-2.331762	-3.652101	0.159167
14	6	0	-2.261657	-4.360747	-1.039268
15	6	0	-2.348022	-3.688639	-2.257426
16	6	0	-2.522139	-2.305052	-2.267124
17	6	0	-2.584647	-1.592730	-1.070475
18	6	0	-0.014320	-1.825498	2.020300
19	8	0	-0.502790	-3.098734	2.451375
20	6	0	0.232501	-4.221209	2.284021
21	8	0	-0.332981	-5.283723	2.370339
22	7	0	-0.301187	1.261631	2.571159
23	6	0	-0.123149	2.597789	2.079798
24	6	0	-0.955419	3.629045	2.504635
25	6	0	-0.806865	4.920714	2.001635
26	6	0	0.215832	5.198852	1.091157
27	6	0	1.092343	4.179200	0.705388
28	6	0	0.920490	2.894736	1.195160
29	8	0	-3.178637	1.938631	1.955038
30	8	0	0.445418	6.418445	0.541869
31	6	0	-0.437158	7.467241	0.891162
32	8	0	-8.621912	-0.506532	-0.418500
33	6	0	-9.165965	0.550965	-1.184249
34	6	0	1.707365	-4.065134	2.036439
35	6	0	0.929204	-5.698883	-1.065867
36	6	0	2.323017	-5.128929	-1.053927
37	8	0	3.312968	-5.758987	-0.784974
38	8	0	2.474220	-3.814851	-1.347673
39	6	0	1.362529	-2.964069	-1.618027
40	6	0	1.895540	-1.561829	-1.629464
41	6	0	3.308420	-1.226281	-1.198416
42	7	0	3.383143	0.210859	-1.456105
43	6	0	2.227147	0.700602	-2.020009
44	6	0	1.286803	-0.464263	-2.108630
45	6	0	4.543873	0.971710	-1.177901
46	6	0	5.790561	0.351594	-1.126025
47	6	0	6.939905	1.074695	-0.809919
48	6	0	6.849208	2.441185	-0.548878
49	6	0	5.599289	3.067418	-0.604287
50	6	0	4.457957	2.345386	-0.907008
51	8	0	7.903500	3.238604	-0.233139
52	6	0	9.179465	2.631989	-0.171572
53	6	0	3.652735	-1.543963	0.249963
54	6	0	4.510989	-2.598141	0.563221
55	6	0	4.889189	-2.827346	1.884688
56	6	0	4.417874	-1.999380	2.901575
57	6	0	3.547724	-0.953225	2.595272
58	6	0	3.165188	-0.732351	1.274836
59	7	0	0.081353	-0.343070	-2.767951
60	6	0	-0.844793	0.687180	-2.453946
61	6	0	-0.784804	1.392129	-1.256571
62	6	0	-1.738801	2.356227	-0.941458
63	6	0	-2.803021	2.583941	-1.815197
64	6	0	-2.877699	1.868335	-3.015361
65	6	0	-1.893484	0.946730	-3.341616
66	8	0	2.015078	1.839812	-2.390782
67	8	0	-3.809400	3.469059	-1.573177
68	6	0	-3.672370	4.293422	-0.424606
69	1	0	4.012498	-1.763302	-1.848201
70	1	0	0.726833	-1.446939	2.734062
71	1	0	0.920593	-3.224872	-2.589319
72	1	0	-2.915871	-2.158616	2.241730
73	1	0	4.873998	-3.247036	-0.229387
74	1	0	5.560642	-3.647859	2.116837
75	1	0	4.726512	-2.166716	3.928678
76	1	0	3.186254	-0.299373	3.384266
77	1	0	2.503694	0.094595	1.021850
78	1	0	-2.275519	-4.183669	1.105031
79	1	0	-2.158950	-5.441747	-1.017283
80	1	0	-2.309452	-4.241312	-3.191350

81	1	0	-2.639047	-1.775914	-3.210155
82	1	0	-2.743199	-0.517636	-1.082648
83	1	0	-5.135247	-2.243346	1.790311
84	1	0	-7.461510	-2.297458	0.937724
85	1	0	-6.881907	1.557632	-0.868584
86	1	0	-4.574133	1.595419	-0.054550
87	1	0	3.498597	2.842912	-0.955965
88	1	0	5.542408	4.130920	-0.396905
89	1	0	7.890840	0.557092	-0.774661
90	1	0	5.884856	-0.710138	-1.327450
91	1	0	0.003259	1.175202	-0.542416
92	1	0	-1.656170	2.897617	-0.005644
93	1	0	-3.705645	2.064240	-3.688643
94	1	0	-1.936152	0.415240	-4.288326
95	1	0	1.600507	2.110508	0.868351
96	1	0	1.888290	4.415201	0.007154
97	1	0	-1.483944	5.697163	2.337701
98	1	0	-1.746421	3.410033	3.209726
99	1	0	0.482395	-1.921670	1.044190
100	1	0	0.573216	-3.093996	-0.859998
101	1	0	1.920382	-3.480250	1.135668
102	1	0	2.172324	-3.528161	2.869047
103	1	0	2.156027	-5.053480	1.938619
104	1	0	0.373042	-5.397183	-1.957060
105	1	0	1.005923	-6.784055	-1.020830
106	1	0	0.368505	-5.352811	-0.189802
107	1	0	0.584096	0.791093	2.723441
108	1	0	-10.191951	0.263575	-1.411652
109	1	0	-9.166174	1.490179	-0.619390
110	1	0	-8.610040	0.690883	-2.118362
111	1	0	-4.537577	4.956318	-0.427552
112	1	0	-3.659355	3.696899	0.494609
113	1	0	-2.751095	4.886592	-0.480896
114	1	0	-0.101117	8.342630	0.336803
115	1	0	-1.468294	7.227835	0.605914
116	1	0	-0.398290	7.677894	1.965853
117	1	0	9.879522	3.424042	0.091902
118	1	0	9.209279	1.848336	0.594235
119	1	0	9.461265	2.202558	-1.139803
120	1	0	-0.371759	-1.229089	-2.970295

4a–R

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	5.336052	-3.566961	-0.024813
2	35	0	-6.943913	-1.707841	0.533151
3	6	0	3.025532	3.062963	2.357271
4	8	0	-0.913931	-0.664719	-0.317687
5	7	0	0.976361	0.656853	-0.552482
6	7	0	-2.313934	1.999508	-0.783199
7	6	0	1.974894	-0.339270	-0.433246
8	6	0	-3.325359	1.069325	-0.476352
9	6	0	2.296115	2.670782	0.089202
10	6	0	4.233348	-1.087226	-0.889607
11	6	0	1.329723	2.044268	-0.895302
12	6	0	-3.400413	0.434489	0.768283
13	6	0	-0.377069	0.411220	-0.486787
14	6	0	1.736311	-1.521243	0.280037
15	6	0	-4.477459	-0.387073	1.071551
16	6	0	-4.358517	0.895192	-1.401369
17	6	0	-1.071257	1.743940	-0.720231
18	6	0	3.293637	3.527367	-0.372910
19	6	0	2.164915	2.440515	1.459701
20	6	0	3.976424	-2.258301	-0.189607
21	6	0	2.736263	-2.478947	0.396756
22	6	0	-5.476560	-0.578786	0.122218
23	6	0	-5.426141	0.052127	-1.114939
24	6	0	3.233268	-0.129652	-1.009011
25	6	0	4.019187	3.925036	1.892875
26	6	0	4.151507	4.157877	0.527155
27	1	0	2.922149	2.875241	3.421301
28	1	0	5.205247	-0.918426	-1.338992

29	1	0	1.772560	2.063981	-1.899595
30	1	0	-2.612814	0.591103	1.498013
31	1	0	0.772786	-1.695782	0.736653
32	1	0	-4.539262	-0.879411	2.035622
33	1	0	-4.310932	1.417613	-2.351129
34	1	0	3.403495	3.699701	-1.441413
35	1	0	1.391898	1.766545	1.820850
36	1	0	2.548727	-3.392833	0.949083
37	1	0	-6.218157	-0.100461	-1.839394
38	1	0	3.452938	0.782104	-1.551391
39	1	0	4.690482	4.409004	2.595064
40	1	0	4.926397	4.822505	0.158592
41	6	0	-0.016272	2.746168	-0.934915
42	6	0	-0.215610	4.050833	-1.100993
43	1	0	-1.226248	4.446704	-1.110624
44	1	0	0.611490	4.744072	-1.221905

4a–S

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	-5.249630	-3.640101	0.066409
2	35	0	7.000550	-1.688104	0.324697
3	6	0	-3.336717	3.133398	2.113201
4	8	0	0.931095	-0.579099	0.081672
5	7	0	-0.957638	0.650863	-0.461417
6	7	0	2.304493	2.077681	-0.499675
7	6	0	-1.941495	-0.358479	-0.332255
8	6	0	3.332387	1.138957	-0.289085
9	6	0	-2.388551	2.649089	-0.053774
10	6	0	-4.129680	-1.214106	-0.920728
11	6	0	-1.317325	2.006499	-0.910660
12	6	0	3.521396	0.037127	-1.130500
13	6	0	0.391432	0.448487	-0.275656
14	6	0	-1.742652	-1.461903	0.506967
15	6	0	4.613761	-0.800566	-0.951815
16	6	0	4.268654	1.408907	0.713026
17	6	0	1.071674	1.778380	-0.560992
18	6	0	-3.363772	3.445217	-0.651551
19	6	0	-2.378131	2.495433	1.333803
20	6	0	-3.911261	-2.309160	-0.094861
21	6	0	-2.726802	-2.436919	0.619718
22	6	0	5.513054	-0.537781	0.076936
23	6	0	5.349576	0.558435	0.915326
24	6	0	-3.145080	-0.240722	-1.037035
25	6	0	-4.308099	3.935213	1.513279
26	6	0	-4.319798	4.091892	0.130480
27	1	0	-3.327214	3.004885	3.190920
28	1	0	-5.059156	-1.117586	-1.470243
29	1	0	-1.665698	1.963037	-1.950861
30	1	0	2.810483	-0.157815	-1.926640
31	1	0	-0.822874	-1.560993	1.065023
32	1	0	4.763649	-1.654815	-1.602447
33	1	0	4.134414	2.284633	1.339378
34	1	0	-3.378973	3.557427	-1.733622
35	1	0	-1.622892	1.868192	1.800995
36	1	0	-2.571007	-3.290885	1.269207
37	1	0	6.065396	0.754511	1.705783
38	1	0	-3.331042	0.611238	-1.680281
39	1	0	-5.055743	4.431648	2.123617
40	1	0	-5.076202	4.709543	-0.343198
41	6	0	0.006962	2.748402	-0.862155
42	6	0	0.182285	4.053982	-1.046293
43	1	0	1.179813	4.478465	-0.992231
44	1	0	-0.652789	4.719990	-1.242095

RCa$_{homo}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.383774	1.496010	-1.574273

2	7	0	0.879010	1.551256	-1.734792
3	6	0	-1.203452	2.682614	-1.293045
4	6	0	-2.612777	2.227869	-0.971049
5	7	0	-2.587509	0.799609	-1.326863
6	6	0	-1.343865	0.321642	-1.669577
7	8	0	-1.065795	-0.818295	-1.991691
8	6	0	-3.724714	-0.017486	-1.120094
9	6	0	-3.681437	3.004748	-1.709359
10	6	0	1.762457	0.484145	-1.980193
11	6	0	1.203435	2.681986	1.293570
12	6	0	0.774418	3.941160	1.347638
13	6	0	-0.774528	3.941829	-1.346878
14	6	0	0.383826	1.495271	1.574528
15	6	0	1.344018	0.320997	1.669876
16	7	0	2.587667	0.799105	1.327341
17	6	0	2.612812	2.227390	0.971600
18	6	0	3.681372	3.004384	1.709929
19	6	0	3.724899	-0.017908	1.120403
20	8	0	1.065978	-0.818990	1.991833
21	6	0	-4.368176	4.022703	-1.049530
22	6	0	-5.315453	4.787533	-1.728461
23	6	0	-5.585445	4.528867	-3.069165
24	6	0	-4.903716	3.506882	-3.730197
25	6	0	-3.952489	2.749891	-3.054735
26	6	0	4.367848	4.022555	1.050153
27	6	0	5.314990	4.787536	1.729099
28	6	0	5.585113	4.528810	3.069766
29	6	0	4.903654	3.506608	3.730741
30	6	0	3.952558	2.749463	3.055264
31	6	0	4.736134	0.420378	0.256615
32	6	0	5.831769	-0.388718	-0.014279
33	6	0	5.923574	-1.637546	0.586323
34	6	0	4.944026	-2.076756	1.467034
35	6	0	3.847893	-1.266629	1.742817
36	6	0	-3.847742	-1.266011	-1.742895
37	6	0	-4.943914	-2.076178	-1.467386
38	6	0	-5.923450	-1.637208	-0.586540
39	6	0	-5.831581	-0.388591	0.014489
40	6	0	-4.735917	0.420550	-0.256147
41	6	0	1.718616	-0.764723	-1.346199
42	6	0	2.720281	-1.701563	-1.566190
43	6	0	3.762665	-1.397982	-2.434759
44	6	0	3.831376	-0.165664	-3.075593
45	6	0	2.844515	0.778160	-2.822756
46	7	0	-0.878993	1.550372	1.734782
47	6	0	-1.762393	0.483202	1.980111
48	6	0	-2.844464	0.777163	2.822681
49	6	0	-3.831340	-0.166663	3.075436
50	6	0	-3.762666	-1.398914	2.434468
51	6	0	-2.720271	-1.702443	1.565897
52	6	0	-1.718533	-0.765638	1.346062
53	35	0	-7.397069	-2.754918	-0.191378
54	35	0	7.397056	-2.755274	0.190683
55	35	0	5.154474	-2.654041	-2.682943
56	35	0	-5.154546	-2.654930	2.682485
57	1	0	-2.771042	2.322889	0.111967
58	1	0	1.439190	4.779831	1.161940
59	1	0	-0.261771	4.146656	1.597233
60	1	0	0.261633	4.147456	-1.596484
61	1	0	-1.439352	4.780412	-1.160960
62	1	0	2.771099	2.322452	-0.111407
63	1	0	-4.164527	4.213948	0.002077
64	1	0	-5.846628	5.577095	-1.206381
65	1	0	-6.328275	5.117402	-3.598161
66	1	0	-5.115051	3.299150	-4.774394
67	1	0	-3.422857	1.951644	-3.568694
68	1	0	4.164095	4.213855	-0.001425
69	1	0	5.845954	5.577267	1.207062
70	1	0	6.327836	5.117467	3.598775
71	1	0	5.115094	3.298832	4.774908
72	1	0	3.423130	1.951052	3.569178
73	1	0	4.672859	1.385033	-0.232151
74	1	0	6.600185	-0.054734	-0.702768
75	1	0	5.032676	-3.048043	1.940752

76	1	0	3.084831	-1.612123	2.424301
77	1	0	-3.084694	-1.611309	-2.424496
78	1	0	-5.032616	-3.047298	-1.941437
79	1	0	-6.599991	-0.054796	0.703077
80	1	0	-4.672625	1.385070	0.232883
81	1	0	0.917703	-1.002747	-0.657843
82	1	0	2.700085	-2.654891	-1.049809
83	1	0	4.659682	0.061533	-3.737512
84	1	0	2.892170	1.760535	-3.282082
85	1	0	-2.892117	1.759507	3.282076
86	1	0	-4.659648	0.060497	3.737368
87	1	0	-2.700088	-2.655724	1.049431
88	1	0	-0.917587	-1.003658	0.657741

RCa_{hetero}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.468563	1.372347	-1.998500
2	7	0	0.793849	1.306817	-2.164115
3	6	0	-1.194058	2.651451	-2.084284
4	6	0	-2.683776	2.370048	-2.072987
5	7	0	-2.738157	0.936414	-1.746424
6	6	0	-1.520795	0.297061	-1.762969
7	8	0	-1.342589	-0.900145	-1.639240
8	6	0	-3.976942	0.274454	-1.564315
9	6	0	-3.455487	3.233085	-1.099015
10	6	0	1.644749	0.191728	-2.093973
11	6	0	0.959411	2.363501	0.967618
12	6	0	0.304572	3.520729	0.898097
13	6	0	-0.625279	3.853995	-2.135955
14	6	0	0.378904	1.074425	1.371727
15	6	0	1.549650	0.142214	1.634930
16	7	0	2.681615	0.797895	1.205100
17	6	0	2.431073	2.149373	0.679436
18	6	0	3.326128	3.205464	1.290820
19	6	0	3.929707	0.166754	0.990837
20	8	0	1.492102	-0.970084	2.124176
21	6	0	-4.245642	4.280252	-1.566343
22	6	0	-4.916318	5.108662	-0.666218
23	6	0	-4.802497	4.884625	0.702346
24	6	0	-4.013492	3.832595	1.170978
25	6	0	-3.340772	3.009631	0.274466
26	6	0	3.753333	4.275215	0.504976
27	6	0	4.525571	5.293136	1.061719
28	6	0	4.881362	5.238451	2.406510
29	6	0	4.460358	4.166220	3.192954
30	6	0	3.682150	3.154880	2.639126
31	6	0	4.831947	0.724131	0.076824
32	6	0	6.025061	0.077126	-0.222327
33	6	0	6.325172	-1.123778	0.403168
34	6	0	5.459226	-1.674444	1.338970
35	6	0	4.267934	-1.028527	1.643047
36	6	0	-4.066371	-0.853796	-0.742855
37	6	0	-5.293365	-1.469752	-0.530095
38	6	0	-6.430717	-0.957822	-1.142477
39	6	0	-6.360782	0.163385	-1.959654
40	6	0	-5.132338	0.780294	-2.167698
41	6	0	1.493866	-0.901000	-1.230579
42	6	0	2.467458	-1.890051	-1.161271
43	6	0	3.585622	-1.806667	-1.984943
44	6	0	3.758639	-0.735233	-2.855904
45	6	0	2.803294	0.271585	-2.883149
46	7	0	-0.877638	0.889835	1.467982
47	6	0	-1.596370	-0.269510	1.803436
48	6	0	-1.251948	-1.587159	1.465495
49	6	0	-2.136674	-2.630068	1.714434
50	6	0	-3.361518	-2.363059	2.317180
51	6	0	-3.719358	-1.070513	2.683494
52	6	0	-2.841736	-0.031776	2.405612
53	35	0	-8.105617	-1.793680	-0.845418
54	35	0	7.906930	-2.049909	-0.059172
55	35	0	4.909594	-3.154703	-1.903296

56	35	0	-4.592262	-3.776732	2.583837
57	1	0	-3.083946	2.524030	-3.084525
58	1	0	0.811070	4.444136	0.631875
59	1	0	-0.757794	3.563522	1.119046
60	1	0	0.457440	3.936590	-2.143660
61	1	0	-1.215807	4.764891	-2.167014
62	1	0	2.571668	2.137552	-0.410811
63	1	0	-4.340957	4.448443	-2.636934
64	1	0	-5.531602	5.922237	-1.037204
65	1	0	-5.328016	5.524664	1.403954
66	1	0	-3.922979	3.656294	2.239005
67	1	0	-2.711936	2.195798	0.630867
68	1	0	3.484049	4.307851	-0.548965
69	1	0	4.854979	6.121465	0.442495
70	1	0	5.489232	6.025680	2.840941
71	1	0	4.739807	4.117841	4.240682
72	1	0	3.355001	2.318240	3.250975
73	1	0	4.613501	1.655902	-0.429380
74	1	0	6.708260	0.503493	-0.948398
75	1	0	5.707685	-2.610609	1.826202
76	1	0	3.594529	-1.461126	2.367170
77	1	0	-3.179080	-1.248214	-0.267120
78	1	0	-5.360728	-2.328183	0.131048
79	1	0	-7.255751	0.556825	-2.427934
80	1	0	-5.088828	1.660370	-2.799305
81	1	0	0.607497	-0.973714	-0.617090
82	1	0	2.357593	-2.717450	-0.468449
83	1	0	4.643470	-0.677939	-3.480156
84	1	0	2.932864	1.136382	-3.526052
85	1	0	-0.302666	-1.806090	0.998912
86	1	0	-1.879859	-3.643807	1.428512
87	1	0	-4.681713	-0.876768	3.143482
88	1	0	-3.115665	0.990665	2.646115

RCa$_{homo}$-in/in

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.733329	1.535456	-1.387565
2	7	0	0.513198	1.328812	-1.532641
3	6	0	-1.295578	2.846636	-1.039540
4	6	0	-2.809699	2.738788	-1.029961
5	7	0	-3.043793	1.303398	-1.276661
6	6	0	-1.904033	0.592538	-1.590385
7	8	0	-1.852631	-0.556980	-1.979042
8	6	0	-4.355861	0.778992	-1.369006
9	6	0	-3.431877	3.246988	0.255586
10	6	0	1.130844	0.095594	-1.799636
11	6	0	1.070671	2.171792	1.937962
12	6	0	0.259409	3.217066	2.093553
13	6	0	-0.582311	3.938222	-0.767352
14	6	0	0.643425	0.765394	1.915500
15	6	0	1.894894	-0.067795	1.686945
16	7	0	2.920525	0.825805	1.472712
17	6	0	2.583116	2.222004	1.786736
18	6	0	3.040453	3.226694	0.750076
19	6	0	4.234985	0.429971	1.129038
20	8	0	1.976977	-1.279009	1.652946
21	6	0	-4.120805	4.458704	0.261172
22	6	0	-4.653013	4.959046	1.449071
23	6	0	-4.502397	4.245967	2.634166
24	6	0	-3.811277	3.033625	2.631420
25	6	0	-3.275067	2.537015	1.447142
26	6	0	3.268927	4.544230	1.149917
27	6	0	3.601689	5.518120	0.211190
28	6	0	3.724878	5.174175	-1.133231
29	6	0	3.520316	3.853991	-1.530870
30	6	0	3.176769	2.882839	-0.593739
31	6	0	5.330256	1.195713	1.538712
32	6	0	6.616968	0.835303	1.154046
33	6	0	6.802622	-0.287786	0.357179
34	6	0	5.722662	-1.055452	-0.063461
35	6	0	4.438548	-0.694756	0.323825

36	6	0	-4.593996	-0.600953	-1.292079
37	6	0	-5.892897	-1.092013	-1.350547
38	6	0	-6.958973	-0.211790	-1.488625
39	6	0	-6.741684	1.156625	-1.570503
40	6	0	-5.443216	1.649632	-1.510868
41	6	0	0.824426	-1.097560	-1.134862
42	6	0	1.601784	-2.231445	-1.334939
43	6	0	2.682269	-2.171354	-2.208165
44	6	0	2.994078	-1.006151	-2.900104
45	6	0	2.225698	0.128605	-2.676878
46	7	0	-0.576758	0.404717	1.986805
47	6	0	-1.038304	-0.920411	2.074229
48	6	0	-2.200835	-1.234144	1.356055
49	6	0	-2.766639	-2.501007	1.432831
50	6	0	-2.190981	-3.444164	2.275804
51	6	0	-1.067688	-3.139173	3.039397
52	6	0	-0.492731	-1.879703	2.935817
53	35	0	-8.727083	-0.886164	-1.565423
54	35	0	8.556592	-0.771660	-0.175085
55	35	0	3.840663	-3.663860	-2.352903
56	35	0	-2.964833	-5.167690	2.409602
57	1	0	-3.218982	3.310909	-1.873059
58	1	0	0.634433	4.236620	2.095815
59	1	0	-0.808819	3.065100	2.214618
60	1	0	0.503533	3.901109	-0.813334
61	1	0	-1.059103	4.875789	-0.493283
62	1	0	3.029866	2.488055	2.754579
63	1	0	-4.246274	5.011220	-0.667175
64	1	0	-5.189864	5.903228	1.443223
65	1	0	-4.921737	4.630319	3.558001
66	1	0	-3.685594	2.474203	3.553340
67	1	0	-2.704205	1.611898	1.456423
68	1	0	3.189376	4.810006	2.202255
69	1	0	3.773693	6.540634	0.531556
70	1	0	3.990807	5.928788	-1.865963
71	1	0	3.629304	3.577677	-2.575656
72	1	0	3.017478	1.855594	-0.905281
73	1	0	5.188250	2.082732	2.146799
74	1	0	7.467629	1.428010	1.470844
75	1	0	5.867618	-1.921595	-0.700797
76	1	0	3.595635	-1.286692	-0.004658
77	1	0	-3.767384	-1.292550	-1.206558
78	1	0	-6.069971	-2.159708	-1.289499
79	1	0	-7.577526	1.838839	-1.678766
80	1	0	-5.295082	2.720314	-1.568695
81	1	0	-0.000058	-1.133057	-0.432398
82	1	0	1.391691	-3.140038	-0.781981
83	1	0	3.847530	-0.975725	-3.568255
84	1	0	2.466918	1.062607	-3.175226
85	1	0	-2.660929	-0.472735	0.734931
86	1	0	-3.657804	-2.742810	0.864522
87	1	0	-0.644865	-3.880880	3.706528
88	1	0	0.381628	-1.635346	3.527428

RCa$_{homo}$–*exo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.646407	-1.073245	-0.959465
2	7	0	-0.599583	-0.834370	-1.088823
3	6	0	1.159573	-2.220190	-0.190734
4	6	0	2.591758	-1.897660	0.191694
5	7	0	2.962040	-0.908475	-0.836890
6	6	0	1.883911	-0.355153	-1.486472
7	8	0	1.929460	0.516648	-2.334346
8	6	0	4.280822	-0.410902	-0.948200
9	6	0	3.497079	-3.105117	0.227903
10	6	0	-1.233696	0.274815	-1.678345
11	6	0	-0.354009	-1.307987	2.871571
12	6	0	0.594926	-2.124118	3.323768
13	6	0	0.514216	-3.357697	0.054083
14	6	0	-1.556114	-1.737409	2.140895
15	6	0	-2.252054	-0.478990	1.651007

16	7	0	-1.504600	0.586231	2.113950
17	6	0	-0.377905	0.207176	2.980155
18	6	0	0.940631	0.840102	2.585804
19	6	0	-1.878233	1.943191	1.955053
20	8	0	-3.294237	-0.417370	1.032809
21	6	0	3.835865	-3.671946	1.454941
22	6	0	4.616380	-4.826107	1.505447
23	6	0	5.068442	-5.410135	0.325939
24	6	0	4.734432	-4.841857	-0.903926
25	6	0	3.947150	-3.696988	-0.953831
26	6	0	1.950277	0.963818	3.541262
27	6	0	3.203019	1.456227	3.179740
28	6	0	3.449296	1.841464	1.863623
29	6	0	2.435292	1.741656	0.911870
30	6	0	1.186171	1.243154	1.273564
31	6	0	-1.427111	2.901683	2.869882
32	6	0	-1.755252	4.242281	2.704676
33	6	0	-2.529043	4.626931	1.617249
34	6	0	-2.977378	3.690743	0.694219
35	6	0	-2.654931	2.349691	0.863450
36	6	0	4.749792	0.112530	-2.158190
37	6	0	6.048609	0.600169	-2.247666
38	6	0	6.878902	0.554575	-1.134586
39	6	0	6.432198	0.024466	0.069775
40	6	0	5.132153	-0.456963	0.161254
41	6	0	-0.701647	1.568596	-1.803030
42	6	0	-1.492550	2.616980	-2.256840
43	6	0	-2.817745	2.378104	-2.600536
44	6	0	-3.367373	1.103527	-2.509600
45	6	0	-2.576534	0.066947	-2.033566
46	7	0	-1.921621	-2.951634	2.054016
47	6	0	-3.012992	-3.397308	1.286080
48	6	0	-3.134388	-3.100094	-0.076010
49	6	0	-4.159263	-3.661149	-0.826110
50	6	0	-5.073500	-4.506431	-0.204852
51	6	0	-4.965082	-4.819216	1.145405
52	6	0	-3.916253	-4.281841	1.882771
53	35	0	8.648398	1.219547	-1.261541
54	35	0	-2.962303	6.456268	1.377812
55	35	0	-3.910979	3.828183	-3.133100
56	35	0	-6.482482	-5.261956	-1.224477
57	1	0	2.592303	-1.403031	1.177410
58	1	0	0.493932	-3.195857	3.179746
59	1	0	1.476415	-1.753619	3.838895
60	1	0	-0.498225	-3.506562	-0.305858
61	1	0	0.986216	-4.169412	0.599862
62	1	0	-0.613430	0.482619	4.017467
63	1	0	3.490538	-3.205525	2.375389
64	1	0	4.875156	-5.261605	2.465312
65	1	0	5.682207	-6.304528	0.362197
66	1	0	5.087929	-5.293436	-1.825402
67	1	0	3.683097	-3.253146	-1.910491
68	1	0	1.755605	0.678423	4.572732
69	1	0	3.982557	1.547615	3.929490
70	1	0	4.424519	2.223343	1.578653
71	1	0	2.620540	2.045292	-0.115996
72	1	0	0.380836	1.187126	0.547002
73	1	0	-0.807237	2.619505	3.713010
74	1	0	-1.403836	4.980725	3.416203
75	1	0	-3.551634	4.001673	-0.173208
76	1	0	-3.001365	1.622146	0.142314
77	1	0	4.102706	0.140796	-3.023811
78	1	0	6.413083	1.006734	-3.184174
79	1	0	7.089804	-0.010811	0.930979
80	1	0	4.784733	-0.859729	1.106063
81	1	0	0.327099	1.771525	-1.542291
82	1	0	-1.084378	3.619328	-2.323197
83	1	0	-4.405245	0.932879	-2.771692
84	1	0	-3.005738	-0.920301	-1.907340
85	1	0	-2.411888	-2.428577	-0.530921
86	1	0	-4.253071	-3.441255	-1.884298
87	1	0	-5.680721	-5.487871	1.610366
88	1	0	-3.795602	-4.534352	2.931099

RCa$_{hetero}$–*exo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.263060	-2.893664	0.118388
2	6	0	3.090337	-3.254993	-1.223547
3	6	0	3.960276	-4.179211	-1.809192
4	6	0	5.028575	-4.695106	-1.084796
5	6	0	5.191866	-4.316305	0.242794
6	6	0	4.312197	-3.428916	0.854396
7	7	0	1.973262	-2.828422	-1.967592
8	6	0	1.661019	-1.607842	-2.134598
9	6	0	0.437036	-1.154420	-2.804719
10	6	0	0.481472	0.359229	-2.917269
11	7	0	1.726376	0.716966	-2.211438
12	6	0	2.465999	-0.368097	-1.793946
13	6	0	-0.539971	-1.951055	-3.231603
14	8	0	3.571212	-0.343433	-1.288070
15	6	0	2.166020	2.062282	-2.146813
16	6	0	1.529641	3.033435	-2.931394
17	6	0	1.922070	4.364779	-2.871529
18	6	0	2.956136	4.736532	-2.023350
19	6	0	3.602244	3.789509	-1.240077
20	6	0	3.212844	2.456461	-1.299071
21	6	0	-0.748893	1.046876	-2.355344
22	6	0	-1.767135	1.437722	-3.225179
23	6	0	-2.906167	2.077271	-2.738246
24	6	0	-3.030028	2.336080	-1.375190
25	6	0	-2.012513	1.948725	-0.502793
26	6	0	-0.880168	1.299033	-0.989091
27	35	0	3.490291	6.551059	-1.934534
28	35	0	6.631185	-5.038982	1.245294
29	7	0	0.442083	-1.192799	1.247591
30	6	0	0.909580	-0.168266	2.093568
31	6	0	1.915101	0.667708	1.598699
32	6	0	2.462365	1.668084	2.394003
33	6	0	2.037929	1.787202	3.711121
34	6	0	1.079139	0.927577	4.241209
35	6	0	0.512990	-0.045929	3.430824
36	35	0	2.793419	3.128721	4.816132
37	6	0	-0.788332	-1.464719	1.061892
38	6	0	-1.263608	-2.611706	0.279578
39	6	0	-2.775196	-2.521818	0.161609
40	7	0	-3.103072	-1.309739	0.928396
41	6	0	-2.018499	-0.685655	1.499000
42	6	0	-0.492396	-3.601213	-0.166336
43	6	0	-3.280705	-2.474372	-1.269702
44	6	0	-3.485242	-3.675665	-1.951971
45	6	0	-3.925172	-3.669175	-3.273105
46	6	0	-4.195284	-2.459622	-3.911424
47	6	0	-4.006903	-1.261020	-3.226770
48	6	0	-3.535449	-1.265193	-1.915750
49	6	0	-4.447809	-0.898412	1.096012
50	6	0	-4.772578	0.415475	1.459904
51	6	0	-6.103370	0.792168	1.599480
52	6	0	-7.112835	-0.133843	1.371409
53	6	0	-6.809074	-1.436920	0.999573
54	6	0	-5.479794	-1.815473	0.860752
55	8	0	-2.035244	0.312167	2.193540
56	35	0	-8.923598	0.387730	1.560148
57	1	0	-3.216747	-3.392167	0.663320
58	1	0	-0.454823	-3.025084	-3.094905
59	1	0	-1.434538	-1.566523	-3.711124
60	1	0	0.574806	-3.590640	0.029321
61	1	0	-0.897315	-4.439084	-0.726362
62	1	0	0.588367	0.637534	-3.974145
63	1	0	-3.311923	-4.622492	-1.445034
64	1	0	-4.076331	-4.608435	-3.795607
65	1	0	-4.559157	-2.453188	-4.934014
66	1	0	-4.217874	-0.313508	-3.713234
67	1	0	-3.377154	-0.324921	-1.393840
68	1	0	-1.663035	1.253894	-4.292702
69	1	0	-3.688665	2.383149	-3.426132

70	1	0	-3.910721	2.843238	-0.993357
71	1	0	-2.088533	2.154251	0.559764
72	1	0	-0.079976	1.020916	-0.306551
73	1	0	0.712962	2.770296	-3.591427
74	1	0	1.419702	5.106120	-3.482310
75	1	0	4.411810	4.085245	-0.582116
76	1	0	3.740837	1.726577	-0.703563
77	1	0	-3.991890	1.138526	1.642553
78	1	0	-6.349781	1.809327	1.882679
79	1	0	-7.600850	-2.154055	0.815699
80	1	0	-5.262532	-2.831825	0.555001
81	1	0	2.270367	0.525060	0.583902
82	1	0	3.221316	2.334085	1.997952
83	1	0	0.774324	1.024732	5.277033
84	1	0	-0.239341	-0.716045	3.831660
85	1	0	3.799273	-4.479244	-2.839456
86	1	0	5.718389	-5.395410	-1.542249
87	1	0	4.449155	-3.154007	1.894347
88	1	0	2.561526	-2.201964	0.577608

RCa$_{hetero}$–*exo'*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.394106	-2.293845	-1.027140
2	7	0	-0.865093	-2.356226	-1.193597
3	6	0	1.153701	-3.332359	-0.316930
4	6	0	2.597872	-2.884457	-0.200045
5	7	0	2.605499	-1.577646	-0.882425
6	6	0	1.398101	-1.240550	-1.465372
7	8	0	1.177061	-0.284091	-2.180558
8	6	0	3.773444	-0.775091	-0.895013
9	6	0	3.570073	-3.879490	-0.804865
10	6	0	-1.703744	-1.386485	-1.766814
11	6	0	-0.792885	-1.705591	2.294542
12	6	0	-0.548161	-2.927177	2.762940
13	6	0	0.645845	-4.467305	0.158313
14	6	0	-2.122973	-1.153251	1.987758
15	6	0	-1.916418	0.312088	1.629839
16	7	0	-0.554676	0.525847	1.635692
17	6	0	0.253691	-0.656707	1.977298
18	6	0	1.240675	-0.378305	3.091091
19	6	0	0.051496	1.737288	1.224313
20	8	0	-2.771238	1.145296	1.411291
21	6	0	4.228730	-4.783547	0.027606
22	6	0	5.075744	-5.748205	-0.514354
23	6	0	5.273099	-5.805216	-1.891300
24	6	0	4.620762	-4.896918	-2.724390
25	6	0	3.769349	-3.938182	-2.184506
26	6	0	0.787836	-0.017070	4.361971
27	6	0	1.698803	0.243580	5.378783
28	6	0	3.070089	0.144250	5.135256
29	6	0	3.526160	-0.211019	3.870118
30	6	0	2.609779	-0.467505	2.851481
31	6	0	1.295067	1.703514	0.583087
32	6	0	1.904045	2.878003	0.159712
33	6	0	1.263581	4.090935	0.376070
34	6	0	0.029789	4.143922	1.013729
35	6	0	-0.576226	2.968945	1.443173
36	6	0	3.866054	0.392955	-1.668118
37	6	0	5.010834	1.180805	-1.607038
38	6	0	6.068248	0.812602	-0.785757
39	6	0	5.999334	-0.347348	-0.025538
40	6	0	4.858823	-1.138323	-0.082841
41	6	0	-1.605722	-0.008290	-1.531525
42	6	0	-2.587324	0.857126	-1.999924
43	6	0	-3.653879	0.344465	-2.731668
44	6	0	-3.761924	-1.017321	-2.997413
45	6	0	-2.799580	-1.878908	-2.489425
46	7	0	-3.202708	-1.817623	2.087654
47	6	0	-4.461194	-1.328964	1.689351
48	6	0	-5.551311	-1.543701	2.537388
49	6	0	-6.826462	-1.138469	2.157921

50	6	0	-7.008699	-0.556445	0.908489
51	6	0	-5.943058	-0.371007	0.032838
52	6	0	-4.672080	-0.761257	0.428470
53	35	0	7.618755	1.893748	-0.708244
54	35	0	2.087749	5.694512	-0.203099
55	35	0	-5.028803	1.505082	-3.319374
56	35	0	-8.748976	-0.019991	0.378021
57	1	0	2.842956	-2.739010	0.861193
58	1	0	-1.368434	-3.615131	2.943091
59	1	0	0.462965	-3.258559	2.981343
60	1	0	-0.411375	-4.678356	0.031366
61	1	0	1.263550	-5.201885	0.666695
62	1	0	0.821393	-0.977573	1.092440
63	1	0	4.083795	-4.728833	1.104615
64	1	0	5.585821	-6.447356	0.140546
65	1	0	5.937367	-6.551308	-2.315340
66	1	0	4.776135	-4.934528	-3.797845
67	1	0	3.265380	-3.229133	-2.836552
68	1	0	-0.280356	0.057263	4.551784
69	1	0	1.341159	0.524510	6.364209
70	1	0	3.778564	0.349398	5.931406
71	1	0	4.590449	-0.278834	3.667177
72	1	0	2.967121	-0.717435	1.854146
73	1	0	1.806316	0.764116	0.402773
74	1	0	2.868099	2.841605	-0.335760
75	1	0	-0.456005	5.098207	1.182902
76	1	0	-1.533951	3.006601	1.942769
77	1	0	3.051270	0.687616	-2.311922
78	1	0	5.074357	2.081839	-2.207299
79	1	0	6.829697	-0.639108	0.607391
80	1	0	4.836785	-2.045988	0.507710
81	1	0	-0.774695	0.391956	-0.962669
82	1	0	-2.530277	1.917040	-1.778596
83	1	0	-4.607263	-1.399483	-3.558458
84	1	0	-2.888139	-2.950309	-2.634903
85	1	0	-5.388893	-2.018121	3.499664
86	1	0	-7.671912	-1.284798	2.820719
87	1	0	-6.095533	0.092765	-0.936916
88	1	0	-3.830415	-0.627606	-0.239804

RCa$_{homo}$-in/in–*exo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.647735	0.225446	-1.928146
2	7	0	0.627094	0.224163	-1.942657
3	6	0	-1.394864	1.383880	-2.465500
4	6	0	-2.880103	1.073042	-2.420692
5	7	0	-2.924780	-0.217315	-1.718680
6	6	0	-1.688735	-0.776500	-1.462004
7	8	0	-1.498798	-1.873191	-0.972006
8	6	0	-4.156789	-0.869665	-1.471909
9	6	0	-3.684481	2.172304	-1.750570
10	6	0	1.603519	-0.685558	-1.525045
11	6	0	1.626519	3.188448	-0.073778
12	6	0	1.690261	4.345914	-0.728155
13	6	0	-0.832410	2.511995	-2.896858
14	6	0	2.765587	2.297327	0.202254
15	6	0	2.208496	1.107968	0.974194
16	7	0	0.845723	1.305177	1.087483
17	6	0	0.369467	2.566543	0.497557
18	6	0	-0.334413	3.489583	1.473129
19	6	0	-0.078013	0.339003	1.548982
20	8	0	2.831305	0.155251	1.398107
21	6	0	-4.046691	3.294324	-2.499473
22	6	0	-4.689563	4.369686	-1.891003
23	6	0	-4.994028	4.324630	-0.531526
24	6	0	-4.665367	3.193092	0.211440
25	6	0	-4.015437	2.122165	-0.397239
26	6	0	0.105913	3.633328	2.788509
27	6	0	-0.536792	4.523376	3.643873
28	6	0	-1.619682	5.276088	3.189510
29	6	0	-2.061953	5.132397	1.876897

30	6	0	-1.421145	4.239159	1.020693
31	6	0	-1.451092	0.624046	1.487046
32	6	0	-2.393430	-0.313327	1.893664
33	6	0	-1.973086	-1.553422	2.351292
34	6	0	-0.620361	-1.850905	2.438892
35	6	0	0.326273	-0.908742	2.054580
36	6	0	-4.270574	-1.853367	-0.480523
37	6	0	-5.501209	-2.441285	-0.215775
38	6	0	-6.619329	-2.059515	-0.946211
39	6	0	-6.524875	-1.086485	-1.932877
40	6	0	-5.296313	-0.490209	-2.191117
41	6	0	1.438527	-1.858813	-0.767827
42	6	0	2.549755	-2.589664	-0.359482
43	6	0	3.823641	-2.169224	-0.724848
44	6	0	4.012853	-1.041267	-1.513305
45	6	0	2.905897	-0.300992	-1.893850
46	7	0	3.932076	2.535808	-0.252952
47	6	0	5.070035	1.723986	-0.142830
48	6	0	5.904003	1.723563	-1.270122
49	6	0	6.999060	0.870334	-1.347731
50	6	0	7.281055	0.046444	-0.263636
51	6	0	6.536794	0.117372	0.910565
52	6	0	5.440418	0.965134	0.976264
53	35	0	-8.296532	-2.863325	-0.584669
54	35	0	-3.262920	-2.848187	2.848605
55	35	0	5.355811	-3.110683	-0.131034
56	35	0	8.681819	-1.217826	-0.385790
57	1	0	-3.244954	0.937202	-3.447811
58	1	0	2.642022	4.699566	-1.111560
59	1	0	0.807845	4.959535	-0.885771
60	1	0	0.249730	2.606980	-2.876765
61	1	0	-1.417230	3.348986	-3.264053
62	1	0	-0.320350	2.329607	-0.320101
63	1	0	-3.827567	3.327132	-3.564319
64	1	0	-4.961039	5.238510	-2.482150
65	1	0	-5.499286	5.160528	-0.057990
66	1	0	-4.911976	3.141040	1.267412
67	1	0	-3.778223	1.232260	0.174975
68	1	0	0.945054	3.040909	3.144772
69	1	0	-0.194120	4.627930	4.668507
70	1	0	-2.120650	5.966645	3.860501
71	1	0	-2.912890	5.703335	1.517639
72	1	0	-1.780343	4.107662	0.000114
73	1	0	-1.804838	1.586756	1.141172
74	1	0	-3.452989	-0.080386	1.855400
75	1	0	-0.297066	-2.818446	2.806766
76	1	0	1.374900	-1.150862	2.126430
77	1	0	-3.404309	-2.160456	0.086093
78	1	0	-5.579620	-3.188318	0.566878
79	1	0	-7.402885	-0.788442	-2.494374
80	1	0	-5.244190	0.280673	-2.951057
81	1	0	0.447351	-2.183312	-0.484460
82	1	0	2.422931	-3.478577	0.249151
83	1	0	5.013627	-0.739851	-1.798351
84	1	0	3.025635	0.608621	-2.475217
85	1	0	5.645869	2.366973	-2.105139
86	1	0	7.612986	0.832420	-2.240630
87	1	0	6.797776	-0.507285	1.757503
88	1	0	4.854076	1.012271	1.882482

TSa$_{homo}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.469502	1.256668	-1.421294
2	7	0	0.816926	1.253200	-1.560933
3	6	0	-1.143931	2.453497	-1.042365
4	6	0	-2.607288	2.176628	-0.830319
5	7	0	-2.723410	0.753382	-1.179154
6	6	0	-1.523888	0.177162	-1.547795
7	8	0	-1.350747	-0.968642	-1.920585
8	6	0	-3.936750	0.055243	-0.972904
9	6	0	-3.486463	3.079971	-1.677771

10	6	0	1.682950	0.182575	-1.785224
11	6	0	1.143902	2.453272	1.042501
12	6	0	0.468747	3.650078	0.877255
13	6	0	-0.468769	3.650277	-0.876959
14	6	0	0.469502	1.256393	1.421312
15	6	0	1.523933	0.176936	1.547862
16	7	0	2.723457	0.753231	1.179331
17	6	0	2.607293	2.176484	0.830532
18	6	0	3.486420	3.079818	1.678042
19	6	0	3.936783	0.055104	0.972961
20	8	0	1.350824	-0.968892	1.920590
21	6	0	-4.032058	4.230712	-1.109458
22	6	0	-4.787897	5.107829	-1.884818
23	6	0	-5.007051	4.832175	-3.231957
24	6	0	-4.466308	3.679614	-3.800930
25	6	0	-3.705105	2.807775	-3.028445
26	6	0	4.031875	4.230680	1.109839
27	6	0	4.787720	5.107752	1.885243
28	6	0	5.007025	4.831937	3.232326
29	6	0	4.466431	3.679256	3.801189
30	6	0	3.705229	2.807456	3.028656
31	6	0	5.008491	0.711273	0.352519
32	6	0	6.189734	0.035793	0.070310
33	6	0	6.310569	-1.302011	0.415189
34	6	0	5.273472	-1.962883	1.059396
35	6	0	4.092752	-1.289604	1.346341
36	6	0	-4.092598	-1.289516	-1.346153
37	6	0	-5.273325	-1.962822	-1.059309
38	6	0	-6.310534	-1.301939	-0.415295
39	6	0	-6.189823	0.035915	-0.070565
40	6	0	-5.008582	0.711432	-0.352695
41	6	0	1.506679	-1.141197	-1.343035
42	6	0	2.518295	-2.076843	-1.502785
43	6	0	3.708910	-1.708507	-2.125710
44	6	0	3.905695	-0.413228	-2.588515
45	6	0	2.902551	0.526840	-2.394067
46	7	0	-0.816940	1.252882	1.560817
47	6	0	-1.682985	0.182266	1.785056
48	6	0	-2.902651	0.526578	2.393741
49	6	0	-3.905810	-0.413478	2.588177
50	6	0	-3.708968	-1.708796	2.125509
51	6	0	-2.518299	-2.077173	1.502710
52	6	0	-1.506677	-1.141533	1.342961
53	35	0	-7.888464	-2.246366	0.027420
54	35	0	7.888508	-2.246377	-0.027599
55	35	0	5.093731	-2.981983	-2.314151
56	35	0	-5.093742	-2.982304	2.314048
57	1	0	-2.857204	2.306167	0.233659
58	1	0	1.042308	4.562998	0.737771
59	1	0	-0.456234	3.744322	1.439598
60	1	0	0.456192	3.744635	-1.439314
61	1	0	-1.042333	4.563167	-0.737274
62	1	0	2.857244	2.306073	-0.233431
63	1	0	-3.870867	4.436761	-0.053212
64	1	0	-5.211401	5.999526	-1.433514
65	1	0	-5.601587	5.509657	-3.836461
66	1	0	-4.638924	3.458453	-4.849466
67	1	0	-3.286405	1.907805	-3.471328
68	1	0	3.870588	4.436864	0.053634
69	1	0	5.211113	5.999540	1.434015
70	1	0	5.601558	5.509389	3.836867
71	1	0	4.639159	3.457963	4.849680
72	1	0	3.286646	1.907397	3.471466
73	1	0	4.934499	1.751878	0.063336
74	1	0	7.004786	0.550587	-0.425921
75	1	0	5.377849	-3.008254	1.328471
76	1	0	3.287964	-1.812409	1.839230
77	1	0	-3.287710	-1.812333	-1.838866
78	1	0	-5.377602	-3.008234	-1.328264
79	1	0	-7.004970	0.550720	0.425501
80	1	0	-4.934671	1.752070	-0.063604
81	1	0	0.579637	-1.435902	-0.871924
82	1	0	2.388829	-3.089459	-1.136588
83	1	0	4.841386	-0.138492	-3.062808

84	1	0	3.040973	1.553254	-2.720431
85	1	0	-3.041102	1.553015	2.720021
86	1	0	-4.841542	-0.138707	3.062367
87	1	0	-2.388788	-3.089823	1.136623
88	1	0	-0.579579	-1.436286	0.871990

TSa$_{hetero}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.691233	1.126381	-1.912828
2	7	0	0.605765	1.056043	-1.916358
3	6	0	-1.332950	2.384399	-1.830727
4	6	0	-2.826334	2.203583	-1.767726
5	7	0	-2.976667	0.743105	-1.801109
6	6	0	-1.772893	0.072946	-1.942862
7	8	0	-1.627531	-1.125644	-2.089669
8	6	0	-4.255467	0.141580	-1.850953
9	6	0	-3.449952	2.891958	-0.565955
10	6	0	1.391731	-0.100610	-1.888165
11	6	0	0.889626	2.451123	0.370775
12	6	0	0.094938	3.565780	0.126261
13	6	0	-0.606083	3.556130	-1.676723
14	6	0	0.397492	1.274079	1.026500
15	6	0	1.597797	0.410657	1.357669
16	7	0	2.698659	1.041618	0.813693
17	6	0	2.382156	2.332900	0.182976
18	6	0	3.149976	3.499260	0.775631
19	6	0	3.951022	0.421077	0.596618
20	8	0	1.566912	-0.654947	1.939187
21	6	0	-3.778679	4.245459	-0.670584
22	6	0	-4.275073	4.935924	0.432758
23	6	0	-4.459733	4.271289	1.643104
24	6	0	-4.153683	2.915276	1.741963
25	6	0	-3.649326	2.226833	0.642105
26	6	0	3.503111	4.567473	-0.049120
27	6	0	4.150715	5.681724	0.480927
28	6	0	4.455567	5.726891	1.838912
29	6	0	4.108431	4.657736	2.664039
30	6	0	3.453943	3.548801	2.136142
31	6	0	4.890319	1.034081	-0.243919
32	6	0	6.059451	0.371159	-0.598744
33	6	0	6.304770	-0.898654	-0.095634
34	6	0	5.428916	-1.483094	0.808911
35	6	0	4.257205	-0.827397	1.160999
36	6	0	-4.429703	-1.240137	-1.676736
37	6	0	-5.704771	-1.793758	-1.706178
38	6	0	-6.810999	-0.979195	-1.906839
39	6	0	-6.658190	0.390071	-2.078134
40	6	0	-5.385928	0.946749	-2.048887
41	6	0	1.129721	-1.253371	-1.127265
42	6	0	2.064666	-2.277910	-1.067657
43	6	0	3.249864	-2.173740	-1.795026
44	6	0	3.528231	-1.051239	-2.563961
45	6	0	2.608889	-0.010702	-2.582817
46	7	0	-0.848452	1.008535	1.185686
47	6	0	-1.304615	-0.083068	1.945087
48	6	0	-2.176732	-1.009230	1.362908
49	6	0	-2.734006	-2.035138	2.120035
50	6	0	-2.440623	-2.113639	3.474262
51	6	0	-1.594402	-1.188685	4.080805
52	6	0	-1.028524	-0.179185	3.316248
53	35	0	-8.545077	-1.740347	-1.946628
54	35	0	7.823074	-1.868030	-0.674191
55	35	0	4.533647	-3.560792	-1.704923
56	35	0	-3.214231	-3.494481	4.519672
57	1	0	-3.270245	2.622760	-2.682663
58	1	0	0.598072	4.524994	0.019764
59	1	0	-0.855764	3.591926	0.655127
60	1	0	0.374640	3.561105	-2.146730
61	1	0	-1.133900	4.506477	-1.666528
62	1	0	2.601221	2.262113	-0.893042
63	1	0	-3.654580	4.760437	-1.621191

64	1	0	-4.526200	5.987976	0.342417
65	1	0	-4.850909	4.805610	2.503057
66	1	0	-4.305594	2.387135	2.678202
67	1	0	-3.411774	1.171873	0.723429
68	1	0	3.274640	4.522436	-1.112586
69	1	0	4.423813	6.507584	-0.168276
70	1	0	4.966652	6.589933	2.253429
71	1	0	4.348797	4.687422	3.722105
72	1	0	3.185588	2.714318	2.778646
73	1	0	4.713970	2.019702	-0.656463
74	1	0	6.763200	0.837279	-1.279372
75	1	0	5.641049	-2.464979	1.216739
76	1	0	3.567777	-1.299907	1.842733
77	1	0	-3.575171	-1.885717	-1.537480
78	1	0	-5.830741	-2.862361	-1.572188
79	1	0	-7.524202	1.023656	-2.231969
80	1	0	-5.292263	2.018717	-2.171727
81	1	0	0.213657	-1.330806	-0.551791
82	1	0	1.879204	-3.151144	-0.452137
83	1	0	4.463393	-0.978826	-3.108132
84	1	0	2.812691	0.892600	-3.149939
85	1	0	-2.402957	-0.940702	0.304133
86	1	0	-3.397889	-2.757612	1.657992
87	1	0	-1.379681	-1.260510	5.141284
88	1	0	-0.367979	0.548483	3.776955

TSa_{homo}-in/in

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.683519	1.503547	-1.236557
2	7	0	0.594549	1.336437	-1.388112
3	6	0	-1.227238	2.692688	-0.694515
4	6	0	-2.730834	2.625624	-0.692199
5	7	0	-2.997440	1.271870	-1.189405
6	6	0	-1.851427	0.609571	-1.599965
7	8	0	-1.806300	-0.461197	-2.171130
8	6	0	-4.317594	0.813205	-1.402818
9	6	0	-3.333539	2.957014	0.661706
10	6	0	1.190012	0.132417	-1.780538
11	6	0	0.907384	2.177390	1.558281
12	6	0	0.032514	3.272447	1.558158
13	6	0	-0.440237	3.718446	-0.156302
14	6	0	0.487182	0.818240	1.621271
15	6	0	1.744932	-0.032068	1.529378
16	7	0	2.793748	0.847553	1.356324
17	6	0	2.416840	2.248302	1.568416
18	6	0	2.987077	3.242367	0.578634
19	6	0	4.121683	0.433676	1.107273
20	8	0	1.823180	-1.243063	1.556479
21	6	0	-3.615561	4.293671	0.952833
22	6	0	-4.083276	4.656519	2.213916
23	6	0	-4.286192	3.680422	3.186541
24	6	0	-4.025202	2.343607	2.890811
25	6	0	-3.547557	1.981379	1.634157
26	6	0	3.140466	4.571190	0.978719
27	6	0	3.575894	5.534132	0.070306
28	6	0	3.879491	5.167845	-1.238513
29	6	0	3.752197	3.836333	-1.632204
30	6	0	3.304841	2.877350	-0.728745
31	6	0	5.199624	1.175733	1.592539
32	6	0	6.502207	0.796119	1.283378
33	6	0	6.717289	-0.323337	0.488719
34	6	0	5.652472	-1.068935	-0.006026
35	6	0	4.354274	-0.688136	0.304639
36	6	0	-4.593211	-0.542464	-1.637575
37	6	0	-5.904977	-0.969368	-1.809978
38	6	0	-6.946132	-0.052616	-1.747895
39	6	0	-6.691957	1.292339	-1.514739
40	6	0	-5.382212	1.722171	-1.342276
41	6	0	0.846793	-1.124635	-1.259633
42	6	0	1.616607	-2.243574	-1.553392
43	6	0	2.722368	-2.111646	-2.386495

44	6	0	3.054407	-0.889160	-2.963077
45	6	0	2.293520	0.226288	-2.647017
46	7	0	-0.757461	0.460659	1.645189
47	6	0	-1.167053	-0.857663	1.884426
48	6	0	-2.223589	-1.384784	1.128124
49	6	0	-2.731861	-2.652726	1.388663
50	6	0	-2.206246	-3.387487	2.442364
51	6	0	-1.180860	-2.874237	3.233775
52	6	0	-0.664246	-1.618989	2.952761
53	35	0	-8.731954	-0.641086	-1.978456
54	35	0	8.491908	-0.833213	0.059403
55	35	0	3.873574	-3.592408	-2.646781
56	35	0	-2.905331	-5.107069	2.824252
57	1	0	-3.111658	3.352071	-1.426665
58	1	0	0.468609	4.231414	1.834866
59	1	0	-0.948402	3.084230	1.991577
60	1	0	0.550684	3.817724	-0.597677
61	1	0	-0.944379	4.661370	0.048508
62	1	0	2.735470	2.557240	2.577312
63	1	0	-3.476885	5.054247	0.186902
64	1	0	-4.298062	5.698149	2.430395
65	1	0	-4.655810	3.958698	4.168329
66	1	0	-4.191574	1.576421	3.640381
67	1	0	-3.337396	0.941350	1.412547
68	1	0	2.926848	4.854077	2.007422
69	1	0	3.688730	6.565189	0.389936
70	1	0	4.226431	5.914102	-1.946135
71	1	0	4.005096	3.542371	-2.646572
72	1	0	3.208508	1.840084	-1.027152
73	1	0	5.031509	2.057411	2.202779
74	1	0	7.342058	1.370728	1.656988
75	1	0	5.821505	-1.930389	-0.644238
76	1	0	3.519112	-1.256759	-0.082895
77	1	0	-3.788423	-1.260554	-1.703876
78	1	0	-6.110969	-2.018292	-1.991737
79	1	0	-7.507962	2.004307	-1.465194
80	1	0	-5.206334	2.773512	-1.149494
81	1	0	0.005637	-1.221344	-0.581730
82	1	0	1.379427	-3.201948	-1.105246
83	1	0	3.914886	-0.807727	-3.617543
84	1	0	2.543518	1.196463	-3.065676
85	1	0	-2.641883	-0.799967	0.317230
86	1	0	-3.537775	-3.055004	0.784602
87	1	0	-0.790242	-3.454809	4.062178
88	1	0	0.130719	-1.212994	3.568539

TSa$_{homo}$–*exo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.101846	-1.261027	0.471851
2	7	0	0.195240	-1.149631	0.600453
3	6	0	-1.637137	-2.168943	-0.464586
4	6	0	-3.117912	-1.956510	-0.604308
5	7	0	-3.413106	-1.056536	0.513778
6	6	0	-2.283738	-0.600661	1.161152
7	8	0	-2.275193	0.160026	2.111620
8	6	0	-4.721043	-0.580495	0.749833
9	6	0	-3.919965	-3.241374	-0.575538
10	6	0	0.929467	-0.253440	1.368607
11	6	0	0.738184	-1.200630	-2.371557
12	6	0	-0.170920	-2.222582	-2.699932
13	6	0	-0.846841	-3.024532	-1.250246
14	6	0	2.022116	-1.434429	-1.793889
15	6	0	2.620746	-0.070522	-1.501591
16	7	0	1.665605	0.862856	-1.861674
17	6	0	0.551427	0.278230	-2.616165
18	6	0	-0.834236	0.798335	-2.285998
19	6	0	1.854107	2.255593	-1.715357
20	8	0	3.708648	0.170832	-1.020581
21	6	0	-4.399646	-3.783160	-1.766549
22	6	0	-5.085941	-4.996629	-1.760242
23	6	0	-5.300909	-5.666340	-0.559174

24	6	0	-4.825129	-5.123307	0.634705
25	6	0	-4.132705	-3.917369	0.627009
26	6	0	-1.846439	0.638227	-3.237003
27	6	0	-3.151875	1.036039	-2.954953
28	6	0	-3.452594	1.616560	-1.723682
29	6	0	-2.438603	1.810988	-0.787320
30	6	0	-1.136115	1.403105	-1.067421
31	6	0	1.291310	3.147910	-2.630745
32	6	0	1.433512	4.519789	-2.447572
33	6	0	2.137609	4.992940	-1.347219
34	6	0	2.698268	4.116880	-0.424347
35	6	0	2.556241	2.748275	-0.609036
36	6	0	-5.103363	-0.090137	2.004844
37	6	0	-6.398181	0.374650	2.206856
38	6	0	-7.315696	0.340105	1.164701
39	6	0	-6.957890	-0.157974	-0.081659
40	6	0	-5.662554	-0.616341	-0.286559
41	6	0	0.500784	0.985193	1.896707
42	6	0	1.404345	1.846476	2.498288
43	6	0	2.744640	1.479515	2.600136
44	6	0	3.190451	0.242539	2.150027
45	6	0	2.283048	-0.607988	1.534559
46	7	0	2.445758	-2.615404	-1.492230
47	6	0	3.704496	-2.900204	-0.956363
48	6	0	3.756973	-3.845973	0.078855
49	6	0	4.971065	-4.230711	0.633872
50	6	0	6.147115	-3.703074	0.113520
51	6	0	6.125158	-2.798447	-0.944413
52	6	0	4.907322	-2.395093	-1.473174
53	35	0	-9.080204	0.971111	1.446982
54	35	0	2.328950	6.861797	-1.095082
55	35	0	3.992175	2.743249	3.249753
56	35	0	7.812660	-4.237983	0.844993
57	1	0	-3.306901	-1.430542	-1.555238
58	1	0	0.317782	-3.124161	-3.068240
59	1	0	-1.037965	-1.932202	-3.290233
60	1	0	0.097149	-3.312539	-0.782304
61	1	0	-1.386663	-3.844917	-1.722122
62	1	0	0.719202	0.459715	-3.691482
63	1	0	-4.240712	-3.250734	-2.702384
64	1	0	-5.458306	-5.411433	-2.691535
65	1	0	-5.841007	-6.607687	-0.550468
66	1	0	-4.993774	-5.641788	1.573194
67	1	0	-3.761221	-3.490776	1.555432
68	1	0	-1.611151	0.210230	-4.208992
69	1	0	-3.929254	0.902751	-3.701111
70	1	0	-4.468103	1.926843	-1.498388
71	1	0	-2.664274	2.262992	0.174374
72	1	0	-0.342806	1.564731	-0.345156
73	1	0	0.731027	2.782036	-3.485051
74	1	0	0.996271	5.213441	-3.156703
75	1	0	3.232139	4.488868	0.444058
76	1	0	2.987792	2.063339	0.108363
77	1	0	-4.392181	-0.068934	2.817777
78	1	0	-6.691110	0.755152	3.178975
79	1	0	-7.681254	-0.188207	-0.888523
80	1	0	-5.393840	-0.998763	-1.264657
81	1	0	-0.537072	1.276978	1.827131
82	1	0	1.077557	2.813790	2.863610
83	1	0	4.236597	-0.030577	2.228521
84	1	0	2.616016	-1.559925	1.132707
85	1	0	2.825131	-4.259376	0.452815
86	1	0	5.004553	-4.942903	1.450730
87	1	0	7.053748	-2.409935	-1.347614
88	1	0	4.882544	-1.688163	-2.294211

TSa_{hetero}–*exo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.778291	-2.325481	-0.564548
2	6	0	3.500903	-2.451636	-1.934052
3	6	0	4.321024	-3.265182	-2.726073

4	6	0	5.435587	-3.890665	-2.181664
5	6	0	5.700058	-3.737164	-0.825157
6	6	0	4.873409	-2.969612	-0.008519
7	7	0	2.351749	-1.911663	-2.523161
8	6	0	1.938916	-0.711724	-2.293488
9	6	0	0.643386	-0.247439	-2.675126
10	6	0	0.539986	1.234034	-2.422817
11	7	0	1.772545	1.524918	-1.674883
12	6	0	2.656649	0.458661	-1.649673
13	6	0	-0.324432	-1.063132	-3.287538
14	8	0	3.800113	0.486951	-1.245198
15	6	0	2.121948	2.842840	-1.295909
16	6	0	1.493395	3.936453	-1.901969
17	6	0	1.804310	5.234316	-1.514459
18	6	0	2.750212	5.442611	-0.519673
19	6	0	3.387737	4.369885	0.090693
20	6	0	3.074619	3.071520	-0.293295
21	6	0	-0.736136	1.761328	-1.788598
22	6	0	-1.657954	2.430340	-2.597591
23	6	0	-2.809611	2.990336	-2.048732
24	6	0	-3.059134	2.869695	-0.683468
25	6	0	-2.147188	2.194717	0.127037
26	6	0	-0.987921	1.649746	-0.421294
27	35	0	3.174395	7.210853	0.011404
28	35	0	7.203699	-4.608355	-0.067834
29	7	0	0.327907	-1.297759	0.118368
30	6	0	0.838775	-0.948650	1.382077
31	6	0	1.714738	0.133337	1.529185
32	6	0	2.314236	0.406474	2.754200
33	6	0	2.063732	-0.428262	3.834751
34	6	0	1.214039	-1.524273	3.710355
35	6	0	0.604208	-1.777957	2.491590
36	35	0	2.896541	-0.078342	5.501019
37	6	0	-0.946980	-1.536122	-0.023148
38	6	0	-1.506208	-2.140866	-1.163682
39	6	0	-3.002804	-2.224288	-1.026550
40	7	0	-3.252751	-1.502435	0.227187
41	6	0	-2.095925	-1.113038	0.873069
42	6	0	-0.752580	-2.500262	-2.289776
43	6	0	-3.712209	-1.637376	-2.230589
44	6	0	-4.186063	-2.484311	-3.231375
45	6	0	-4.755186	-1.952893	-4.387609
46	6	0	-4.858076	-0.572883	-4.539882
47	6	0	-4.388512	0.274001	-3.535584
48	6	0	-3.812052	-0.254781	-2.384922
49	6	0	-4.564936	-1.284275	0.701823
50	6	0	-4.850929	-0.255058	1.608337
51	6	0	-6.155776	-0.050697	2.041331
52	6	0	-7.177559	-0.863126	1.566364
53	6	0	-6.912643	-1.882242	0.660961
54	6	0	-5.608062	-2.091228	0.231432
55	8	0	-2.018050	-0.498506	1.918811
56	35	0	-8.955958	-0.571933	2.152829
57	1	0	-3.302382	-3.276504	-0.913296
58	1	0	0.100248	-1.697216	-4.067995
59	1	0	-1.259309	-0.581576	-3.574708
60	1	0	0.272766	-2.821592	-2.082444
61	1	0	-1.273504	-3.111962	-3.025545
62	1	0	0.621556	1.715063	-3.411973
63	1	0	-4.113372	-3.562392	-3.104811
64	1	0	-5.123428	-2.617371	-5.162724
65	1	0	-5.307180	-0.156537	-5.435955
66	1	0	-4.470149	1.350598	-3.647735
67	1	0	-3.441262	0.401511	-1.600573
68	1	0	-1.461786	2.534951	-3.662880
69	1	0	-3.505716	3.526339	-2.686642
70	1	0	-3.955248	3.303820	-0.251489
71	1	0	-2.323042	2.095899	1.193401
72	1	0	-0.270674	1.160301	0.228515
73	1	0	0.752035	3.791384	-2.678342
74	1	0	1.311525	6.076138	-1.987290
75	1	0	4.125174	4.542010	0.866547
76	1	0	3.586689	2.241177	0.173497
77	1	0	-4.056638	0.376731	1.978321

78	1	0	-6.374346	0.746040	2.743490
79	1	0	-7.715331	-2.510132	0.291237
80	1	0	-5.415761	-2.887148	-0.478668
81	1	0	1.901191	0.788709	0.687304
82	1	0	2.974465	1.260263	2.861776
83	1	0	1.032109	-2.172480	4.560388
84	1	0	-0.050910	-2.636613	2.382171
85	1	0	4.079977	-3.387492	-3.777010
86	1	0	6.083729	-4.502350	-2.799124
87	1	0	5.085798	-2.877062	1.050828
88	1	0	3.118749	-1.733304	0.061930

TSa$_{hetero}$–exo'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.490742	-1.738569	-1.293722
2	7	0	-0.792420	-1.522288	-1.355132
3	6	0	0.957634	-2.888690	-0.618019
4	6	0	2.450647	-2.829033	-0.452533
5	7	0	2.788546	-1.520993	-1.029474
6	6	0	1.709054	-0.910591	-1.652198
7	8	0	1.751108	0.098029	-2.329273
8	6	0	4.072497	-0.953273	-0.861152
9	6	0	3.147362	-3.995626	-1.137100
10	6	0	-1.514921	-0.410779	-1.772236
11	6	0	-0.917034	-1.666743	1.457455
12	6	0	-0.597693	-3.017793	1.604191
13	6	0	0.073392	-3.774170	0.004030
14	6	0	-2.212185	-1.068752	1.244575
15	6	0	-1.963029	0.436542	1.146985
16	7	0	-0.602664	0.627437	1.286818
17	6	0	0.132597	-0.609416	1.554687
18	6	0	0.888373	-0.581973	2.871586
19	6	0	0.079551	1.845634	1.067053
20	8	0	-2.780887	1.319085	0.975770
21	6	0	3.514152	-5.110287	-0.383557
22	6	0	4.095405	-6.214931	-1.002911
23	6	0	4.316865	-6.204944	-2.377524
24	6	0	3.954198	-5.089061	-3.130877
25	6	0	3.367689	-3.988032	-2.514488
26	6	0	0.209200	-0.344326	4.068190
27	6	0	0.900974	-0.341581	5.273853
28	6	0	2.276239	-0.580269	5.293451
29	6	0	2.957553	-0.816008	4.103579
30	6	0	2.262717	-0.813245	2.894795
31	6	0	1.442198	1.819423	0.736625
32	6	0	2.134670	2.995716	0.478510
33	6	0	1.466108	4.210245	0.550974
34	6	0	0.118856	4.258105	0.886320
35	6	0	-0.574992	3.082298	1.148974
36	6	0	4.374576	0.344575	-1.305913
37	6	0	5.625981	0.895384	-1.055138
38	6	0	6.586240	0.162257	-0.369762
39	6	0	6.308021	-1.124359	0.069706
40	6	0	5.057007	-1.678929	-0.174100
41	6	0	-1.059100	0.918044	-1.880796
42	6	0	-1.956963	1.948750	-2.120671
43	6	0	-3.310155	1.661709	-2.278856
44	6	0	-3.784868	0.356557	-2.220382
45	6	0	-2.888262	-0.664833	-1.948458
46	7	0	-3.273486	-1.791389	1.178763
47	6	0	-4.619710	-1.488507	0.987483
48	6	0	-5.467983	-2.599812	1.161267
49	6	0	-6.841845	-2.503516	1.002720
50	6	0	-7.386584	-1.274519	0.644691
51	6	0	-6.578506	-0.158380	0.450834
52	6	0	-5.203927	-0.258014	0.625419
53	35	0	8.288177	0.921484	-0.035585
54	35	0	2.403842	5.817189	0.194958
55	35	0	-4.542095	3.077597	-2.519762
56	35	0	-9.258903	-1.118491	0.410778
57	1	0	2.710908	-2.838388	0.616510

58	1	0	-1.442005	-3.686475	1.754676
59	1	0	0.269410	-3.230335	2.227458
60	1	0	-0.892737	-3.858957	-0.488106
61	1	0	0.477765	-4.702508	0.401998
62	1	0	0.873351	-0.799498	0.761789
63	1	0	3.352381	-5.112022	0.692558
64	1	0	4.381324	-7.077524	-0.409517
65	1	0	4.775143	-7.061706	-2.860957
66	1	0	4.129107	-5.075323	-4.201906
67	1	0	3.088854	-3.117881	-3.103196
68	1	0	-0.862551	-0.160097	4.051369
69	1	0	0.368428	-0.154563	6.200813
70	1	0	2.813847	-0.576719	6.236196
71	1	0	4.028540	-0.991404	4.109766
72	1	0	2.801800	-0.972200	1.960920
73	1	0	1.989589	0.885905	0.669331
74	1	0	3.187640	2.958601	0.221075
75	1	0	-0.393615	5.211645	0.948247
76	1	0	-1.622739	3.124470	1.405844
77	1	0	3.639128	0.921149	-1.846658
78	1	0	5.849330	1.899048	-1.399944
79	1	0	7.059994	-1.698053	0.599577
80	1	0	4.868997	-2.688642	0.169304
81	1	0	-0.011553	1.150735	-1.744192
82	1	0	-1.609485	2.975326	-2.161801
83	1	0	-4.842226	0.149366	-2.342741
84	1	0	-3.234358	-1.688141	-1.843448
85	1	0	-5.011713	-3.547529	1.426921
86	1	0	-7.481286	-3.367081	1.146433
87	1	0	-7.021002	0.789409	0.163311
88	1	0	-4.584019	0.613214	0.470620

TSa$_{homo}$-in/in–*exo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.406410	0.358695	-1.894146
2	7	0	0.896499	0.294359	-1.924801
3	6	0	-1.029653	1.568985	-2.276818
4	6	0	-2.533780	1.415584	-2.217137
5	7	0	-2.693546	0.054096	-1.690039
6	6	0	-1.495393	-0.612036	-1.499097
7	8	0	-1.377927	-1.760621	-1.117147
8	6	0	-3.964583	-0.554198	-1.558018
9	6	0	-3.270930	2.473663	-1.409107
10	6	0	1.802045	-0.698617	-1.589087
11	6	0	1.029331	2.596802	-0.251400
12	6	0	0.721711	3.506213	-1.270327
13	6	0	-0.242740	2.677635	-2.650107
14	6	0	2.268252	1.947220	0.095552
15	6	0	1.873883	0.807587	1.052020
16	7	0	0.515575	0.928351	1.275307
17	6	0	-0.045229	2.127686	0.665115
18	6	0	-0.446056	3.201904	1.672150
19	6	0	-0.350321	-0.069897	1.770789
20	8	0	2.578760	-0.073948	1.496994
21	6	0	-3.419480	3.751520	-1.955784
22	6	0	-4.076437	4.753299	-1.243902
23	6	0	-4.614316	4.480262	0.012843
24	6	0	-4.484968	3.203817	0.554411
25	6	0	-3.814170	2.206519	-0.150256
26	6	0	0.157712	3.266320	2.928442
27	6	0	-0.189220	4.279859	3.817945
28	6	0	-1.137741	5.235865	3.459251
29	6	0	-1.741632	5.172054	2.205963
30	6	0	-1.397743	4.157950	1.315822
31	6	0	-1.705386	0.251911	1.938164
32	6	0	-2.639181	-0.736073	2.221156
33	6	0	-2.216496	-2.051331	2.354322
34	6	0	-0.867273	-2.374059	2.284251
35	6	0	0.071323	-1.385502	2.009745
36	6	0	-4.163637	-1.627578	-0.678116
37	6	0	-5.430494	-2.176488	-0.520669

38	6	0	-6.500221	-1.661835	-1.242161
39	6	0	-6.321728	-0.596504	-2.115202
40	6	0	-5.055976	-0.042709	-2.268892
41	6	0	1.588353	-1.874575	-0.839111
42	6	0	2.668592	-2.641552	-0.421895
43	6	0	3.963511	-2.257432	-0.767205
44	6	0	4.195761	-1.163963	-1.589724
45	6	0	3.118133	-0.391101	-1.985226
46	7	0	3.394771	2.284622	-0.428051
47	6	0	4.648617	1.704321	-0.225370
48	6	0	5.541397	1.855690	-1.301065
49	6	0	6.752509	1.177456	-1.332351
50	6	0	7.091144	0.366184	-0.253107
51	6	0	6.290020	0.309381	0.882758
52	6	0	5.082368	0.993216	0.905936
53	35	0	-8.226321	-2.413016	-1.023296
54	35	0	-3.510117	-3.416599	2.575011
55	35	0	5.465479	-3.185450	-0.084703
56	35	0	8.633853	-0.723581	-0.345199
57	1	0	-2.917894	1.448364	-3.247929
58	1	0	1.569100	3.917669	-1.813135
59	1	0	-0.040035	4.242850	-1.017754
60	1	0	0.658827	2.373151	-3.178166
61	1	0	-0.751224	3.534892	-3.083343
62	1	0	-0.930063	1.855474	0.059194
63	1	0	-3.039973	3.960849	-2.952999
64	1	0	-4.181761	5.741563	-1.680039
65	1	0	-5.137760	5.256203	0.562381
66	1	0	-4.905762	2.979160	1.529511
67	1	0	-3.729065	1.211259	0.273794
68	1	0	0.890472	2.518246	3.217244
69	1	0	0.282002	4.319735	4.794914
70	1	0	-1.408448	6.022634	4.156127
71	1	0	-2.490424	5.903871	1.917919
72	1	0	-1.884224	4.105203	0.344867
73	1	0	-2.045427	1.276584	1.842559
74	1	0	-3.690717	-0.484889	2.315906
75	1	0	-0.545373	-3.400827	2.418896
76	1	0	1.118464	-1.641499	1.936071
77	1	0	-3.336361	-2.034039	-0.114449
78	1	0	-5.574135	-2.995569	0.175883
79	1	0	-7.162162	-0.196018	-2.670678
80	1	0	-4.935289	0.798690	-2.941808
81	1	0	0.582453	-2.154735	-0.554749
82	1	0	2.509071	-3.518086	0.197391
83	1	0	5.208636	-0.897500	-1.869204
84	1	0	3.271242	0.504641	-2.578235
85	1	0	5.230334	2.465536	-2.143377
86	1	0	7.408872	1.249168	-2.192600
87	1	0	6.594401	-0.291312	1.732655
88	1	0	4.460386	0.935041	1.785825

5a$_{homo}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.400219	1.443511	-1.278816
2	7	0	0.928380	1.378254	-0.878953
3	6	0	-1.193497	2.471211	-0.950258
4	6	0	-2.635247	2.068039	-1.062800
5	7	0	-2.562092	0.693650	-1.563228
6	6	0	-1.239333	0.271616	-1.659304
7	8	0	-0.855430	-0.851011	-1.932210
8	6	0	-3.655682	-0.188821	-1.419424
9	6	0	-3.474904	2.990202	-1.921932
10	6	0	1.939532	0.584851	-1.505620
11	6	0	1.158128	2.115306	0.415892
12	6	0	0.719600	3.569630	0.255129
13	6	0	-0.735761	3.707372	-0.254757
14	6	0	0.380934	1.246999	1.386206
15	6	0	1.316754	0.118368	1.779969
16	7	0	2.584245	0.530218	1.422778
17	6	0	2.608285	1.902879	0.888474

18	6	0	3.077905	2.921648	1.906807
19	6	0	3.727555	-0.296730	1.329742
20	8	0	1.006461	-0.920106	2.330536
21	6	0	-4.303775	3.936826	-1.322211
22	6	0	-5.036409	4.827043	-2.105747
23	6	0	-4.944798	4.768620	-3.493416
24	6	0	-4.116749	3.821063	-4.096155
25	6	0	-3.381148	2.937583	-3.313688
26	6	0	3.824262	4.018505	1.470772
27	6	0	4.227057	5.001201	2.370764
28	6	0	3.888826	4.890654	3.717678
29	6	0	3.151297	3.794128	4.159283
30	6	0	2.747915	2.811668	3.258527
31	6	0	4.937448	0.259138	0.891578
32	6	0	6.022445	-0.554680	0.589503
33	6	0	5.912335	-1.928532	0.752135
34	6	0	4.747180	-2.489140	1.259853
35	6	0	3.656793	-1.679530	1.555407
36	6	0	-3.610064	-1.494040	-1.929343
37	6	0	-4.646304	-2.383846	-1.667156
38	6	0	-5.740713	-1.972607	-0.918024
39	6	0	-5.829395	-0.667149	-0.454041
40	6	0	-4.792773	0.221710	-0.708886
41	6	0	2.026553	-0.792268	-1.290643
42	6	0	3.128867	-1.508579	-1.743479
43	6	0	4.151824	-0.834782	-2.400145
44	6	0	4.059128	0.523341	-2.684009
45	6	0	2.940992	1.225260	-2.242278
46	7	0	-0.850677	1.427653	1.628843
47	6	0	-1.780386	0.456296	2.042245
48	6	0	-2.821245	0.848929	2.892388
49	6	0	-3.902739	0.005681	3.119224
50	6	0	-3.960411	-1.216928	2.457522
51	6	0	-2.939554	-1.625018	1.606646
52	6	0	-1.847022	-0.791414	1.406937
53	35	0	-7.124660	-3.201911	-0.520338
54	35	0	7.360141	-3.044045	0.265623
55	35	0	5.731062	-1.778079	-2.843581
56	35	0	-5.488468	-2.318284	2.648228
57	1	0	-3.032786	2.056561	-0.035764
58	1	0	1.416026	4.035439	-0.451769
59	1	0	0.827799	4.092245	1.209048
60	1	0	-0.816500	4.578057	-0.916298
61	1	0	-1.411116	3.889422	0.587876
62	1	0	3.273056	1.937233	0.025051
63	1	0	-4.379917	3.973978	-0.237406
64	1	0	-5.682458	5.558789	-1.631079
65	1	0	-5.519408	5.456197	-4.105923
66	1	0	-4.045100	3.771481	-5.178132
67	1	0	-2.734755	2.196827	-3.777318
68	1	0	4.091548	4.102010	0.419252
69	1	0	4.809623	5.847534	2.021200
70	1	0	4.205086	5.652738	4.422695
71	1	0	2.892458	3.698895	5.208922
72	1	0	2.186461	1.953093	3.616923
73	1	0	5.050344	1.330477	0.774952
74	1	0	6.943513	-0.118673	0.219157
75	1	0	4.678484	-3.561240	1.407712
76	1	0	2.744498	-2.124639	1.924389
77	1	0	-2.756146	-1.821004	-2.503515
78	1	0	-4.596111	-3.398635	-2.046261
79	1	0	-6.690970	-0.347926	0.121848
80	1	0	-4.882776	1.233287	-0.332358
81	1	0	1.247416	-1.296027	-0.728652
82	1	0	3.218144	-2.569420	-1.538435
83	1	0	4.857149	1.028233	-3.216538
84	1	0	2.857719	2.292766	-2.427524
85	1	0	-2.782648	1.829355	3.356493
86	1	0	-4.710947	0.309731	3.775025
87	1	0	-3.013583	-2.569651	1.078601
88	1	0	-1.064898	-1.086739	0.714257

$5a_{hetero}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.415230	0.975769	-1.851767
2	7	0	0.905177	1.055695	-1.389124
3	6	0	-1.060150	2.116060	-2.122033
4	6	0	-2.520387	1.863550	-2.383577
5	7	0	-2.626147	0.427400	-2.092755
6	6	0	-1.406209	-0.136182	-1.756094
7	8	0	-1.232745	-1.293983	-1.416852
8	6	0	-3.871267	-0.208797	-1.878384
9	6	0	-3.432460	2.737028	-1.546720
10	6	0	1.888327	0.049790	-1.653881
11	6	0	0.997576	1.961977	-0.174819
12	6	0	0.254282	3.291976	-0.440310
13	6	0	-0.339546	3.393022	-1.868962
14	6	0	0.403622	1.096470	0.928022
15	6	0	1.544783	0.284572	1.515084
16	7	0	2.701357	0.838144	1.021816
17	6	0	2.473314	2.087084	0.276372
18	6	0	2.772312	3.310640	1.122365
19	6	0	3.976977	0.230259	1.043792
20	8	0	1.449843	-0.653735	2.283217
21	6	0	-4.050175	3.844075	-2.125851
22	6	0	-4.850607	4.685863	-1.354671
23	6	0	-5.044690	4.414779	-0.003289
24	6	0	-4.431992	3.303438	0.576206
25	6	0	-3.623772	2.470723	-0.190087
26	6	0	3.442587	4.392740	0.548176
27	6	0	3.694211	5.543977	1.290202
28	6	0	3.277957	5.619902	2.617172
29	6	0	2.614130	4.540929	3.197477
30	6	0	2.364451	3.389881	2.455110
31	6	0	5.094564	0.967210	0.634380
32	6	0	6.325523	0.344199	0.461391
33	6	0	6.443076	-1.014448	0.717607
34	6	0	5.360861	-1.745617	1.191908
35	6	0	4.129804	-1.127321	1.361929
36	6	0	-4.063965	-1.008029	-0.746926
37	6	0	-5.306698	-1.570173	-0.486775
38	6	0	-6.358946	-1.320255	-1.361644
39	6	0	-6.187773	-0.520606	-2.485165
40	6	0	-4.937695	0.034332	-2.743546
41	6	0	1.771886	-1.271791	-1.208266
42	6	0	2.818551	-2.169373	-1.388985
43	6	0	3.991520	-1.739408	-2.002334
44	6	0	4.109354	-0.450082	-2.502314
45	6	0	3.044298	0.432463	-2.340910
46	7	0	-0.841864	1.054143	1.152276
47	6	0	-1.566906	0.067717	1.845419
48	6	0	-1.336745	-1.304938	1.683334
49	6	0	-2.262752	-2.230368	2.149541
50	6	0	-3.415986	-1.782024	2.785252
51	6	0	-3.641739	-0.426927	3.003432
52	6	0	-2.718197	0.491919	2.522275
53	35	0	-8.063779	-2.069866	-1.003631
54	35	0	8.083654	-1.895278	0.386555
55	35	0	5.469528	-2.916041	-2.114761
56	35	0	-4.739585	-3.037135	3.295408
57	1	0	-2.738021	2.047915	-3.445803
58	1	0	0.919328	4.140177	-0.265209
59	1	0	-0.569704	3.363255	0.276116
60	1	0	0.477058	3.505791	-2.591802
61	1	0	-0.990754	4.267545	-1.941654
62	1	0	3.121698	2.097709	-0.601897
63	1	0	-3.908647	4.047303	-3.184773
64	1	0	-5.329563	5.544955	-1.813721
65	1	0	-5.676273	5.062267	0.596712
66	1	0	-4.591709	3.083271	1.627763
67	1	0	-3.141410	1.605630	0.254071
68	1	0	3.767378	4.333088	-0.488754
69	1	0	4.219074	6.376796	0.833317
70	1	0	3.475264	6.514132	3.199528
71	1	0	2.293521	4.591787	4.233009

72	1	0	1.859565	2.550347	2.926100
73	1	0	5.014959	2.029990	0.435794
74	1	0	7.181621	0.914059	0.118461
75	1	0	5.468490	-2.804490	1.399725
76	1	0	3.284031	-1.704403	1.707014
77	1	0	-3.240295	-1.180190	-0.064853
78	1	0	-5.453875	-2.170604	0.406164
79	1	0	-7.020646	-0.331659	-3.152914
80	1	0	-4.796341	0.661936	-3.618112
81	1	0	0.857193	-1.591672	-0.723092
82	1	0	2.738708	-3.186527	-1.021061
83	1	0	5.020173	-0.136008	-2.999749
84	1	0	3.110335	1.441204	-2.737844
85	1	0	-0.460007	-1.645064	1.148612
86	1	0	-2.105224	-3.291190	1.990041
87	1	0	-4.543430	-0.095759	3.505995
88	1	0	-2.893063	1.557614	2.636601

5a$_{homo}$-in/in

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.716701	-0.384549	-0.475086
2	7	0	-0.450115	-0.143158	0.041754
3	6	0	-2.025845	-0.569551	-1.766179
4	6	0	-3.518533	-0.617062	-1.948294
5	7	0	-4.013119	-0.461815	-0.579580
6	6	0	-2.978150	-0.255330	0.320528
7	8	0	-3.080382	-0.000846	1.504485
8	6	0	-5.389675	-0.470922	-0.276685
9	6	0	-3.996894	0.483834	-2.880459
10	6	0	-0.144197	-0.589003	1.361077
11	6	0	0.624933	0.100237	-0.931644
12	6	0	0.041330	0.534624	-2.297757
13	6	0	-1.002710	-0.442974	-2.843094
14	6	0	1.531739	1.249568	-0.512699
15	6	0	2.972641	0.796469	-0.576111
16	7	0	2.961383	-0.513106	-0.987633
17	6	0	1.625111	-1.099962	-1.174989
18	6	0	1.429197	-2.362451	-0.356732
19	6	0	4.128561	-1.260378	-1.294483
20	8	0	3.943492	1.476654	-0.309635
21	6	0	-4.420440	0.175847	-4.171612
22	6	0	-4.797574	1.191863	-5.049198
23	6	0	-4.754000	2.519610	-4.634754
24	6	0	-4.328965	2.830775	-3.342619
25	6	0	-3.947123	1.817594	-2.470123
26	6	0	0.459841	-3.279024	-0.764694
27	6	0	0.236773	-4.443414	-0.032871
28	6	0	0.989834	-4.702483	1.109190
29	6	0	1.969277	-3.796070	1.512787
30	6	0	2.192103	-2.635099	0.780401
31	6	0	4.030458	-2.378653	-2.131850
32	6	0	5.157504	-3.126204	-2.448398
33	6	0	6.389598	-2.761870	-1.921474
34	6	0	6.503019	-1.666705	-1.075454
35	6	0	5.376237	-0.917213	-0.756807
36	6	0	-5.880060	-0.029542	0.961420
37	6	0	-7.245530	-0.053925	1.220922
38	6	0	-8.129981	-0.508105	0.251662
39	6	0	-7.663874	-0.942005	-0.981773
40	6	0	-6.299412	-0.924607	-1.242193
41	6	0	0.808170	0.054675	2.156465
42	6	0	1.171881	-0.473930	3.393889
43	6	0	0.556661	-1.627174	3.852298
44	6	0	-0.440299	-2.247607	3.105660
45	6	0	-0.777590	-1.732411	1.866222
46	7	0	1.059106	2.379605	-0.205557
47	6	0	1.838973	3.512349	0.111365
48	6	0	1.605712	4.134913	1.339631
49	6	0	2.292787	5.295687	1.679069
50	6	0	3.174642	5.851722	0.760730
51	6	0	3.386417	5.266293	-0.484099

52	6	0	2.720429	4.091654	-0.805721
53	35	0	-9.991310	-0.530348	0.611981
54	35	0	7.927999	-3.779493	-2.350609
55	35	0	1.100890	-2.393951	5.498411
56	35	0	4.096185	7.448899	1.202341
57	1	0	-3.822129	-1.593146	-2.350531
58	1	0	0.879439	0.662192	-2.991249
59	1	0	-0.428340	1.513612	-2.157767
60	1	0	-0.553560	-1.408714	-3.111256
61	1	0	-1.448946	-0.039555	-3.758047
62	1	0	1.521032	-1.379229	-2.230558
63	1	0	-4.459521	-0.863210	-4.492127
64	1	0	-5.129875	0.943031	-6.052067
65	1	0	-5.051747	3.311788	-5.314260
66	1	0	-4.294355	3.865007	-3.015294
67	1	0	-3.614763	2.059308	-1.463016
68	1	0	-0.130785	-3.082762	-1.657253
69	1	0	-0.522310	-5.147824	-0.358523
70	1	0	0.816412	-5.607842	1.682382
71	1	0	2.550807	-3.983762	2.410483
72	1	0	2.952296	-1.930601	1.105071
73	1	0	3.076782	-2.691534	-2.538878
74	1	0	5.072346	-3.989407	-3.098477
75	1	0	7.466186	-1.397439	-0.656786
76	1	0	5.469033	-0.069225	-0.094978
77	1	0	-5.197309	0.328997	1.716959
78	1	0	-7.617183	0.288489	2.180382
79	1	0	-8.356889	-1.292945	-1.738021
80	1	0	-5.956435	-1.265014	-2.211619
81	1	0	1.275122	0.976598	1.839871
82	1	0	1.929004	0.019630	3.992887
83	1	0	-0.915873	-3.151596	3.469808
84	1	0	-1.503810	-2.258652	1.256442
85	1	0	0.886361	3.701029	2.027105
86	1	0	2.130079	5.771225	2.639706
87	1	0	4.071401	5.720823	-1.190968
88	1	0	2.882501	3.617897	-1.768243

$5a_{homo}$–*exo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.405378	-0.624122	0.630511
2	7	0	0.057336	-0.460831	0.323535
3	6	0	1.965301	-0.572319	1.841686
4	6	0	3.464817	-0.567512	1.709441
5	7	0	3.664256	-0.648943	0.259395
6	6	0	2.455403	-0.641742	-0.422384
7	8	0	2.280919	-0.628597	-1.625699
8	6	0	4.940293	-0.555003	-0.325407
9	6	0	4.101442	-1.711554	2.475827
10	6	0	-0.519068	-1.421261	-0.566044
11	6	0	-0.738406	0.031972	1.480505
12	6	0	-0.303498	-0.653201	2.787384
13	6	0	1.185216	-0.460958	3.104388
14	6	0	-2.211131	-0.212585	1.201853
15	6	0	-2.774286	1.022185	0.528208
16	7	0	-1.825754	2.001237	0.685459
17	6	0	-0.682522	1.603352	1.529809
18	6	0	0.617709	2.226343	1.074903
19	6	0	-2.040545	3.344238	0.288307
20	8	0	-3.833735	1.111443	-0.057210
21	6	0	4.691955	-1.475646	3.716050
22	6	0	5.219608	-2.533010	4.455651
23	6	0	5.161236	-3.829884	3.953345
24	6	0	4.570303	-4.068386	2.712253
25	6	0	4.037459	-3.014009	1.978251
26	6	0	1.510865	2.726959	2.022389
27	6	0	2.776255	3.167875	1.639426
28	6	0	3.148373	3.126861	0.297556
29	6	0	2.236898	2.683276	-0.660516
30	6	0	0.973217	2.246598	-0.276219
31	6	0	-1.611568	4.390989	1.107634

32	6	0	-1.809982	5.710125	0.718423
33	6	0	-2.444255	5.974389	-0.489412
34	6	0	-2.877145	4.943013	-1.314457
35	6	0	-2.670264	3.624202	-0.927340
36	6	0	5.143390	-0.834158	-1.685280
37	6	0	6.415031	-0.734713	-2.236586
38	6	0	7.490882	-0.367235	-1.438337
39	6	0	7.310864	-0.098184	-0.088666
40	6	0	6.039298	-0.190669	0.464321
41	6	0	-1.403866	-0.990073	-1.555376
42	6	0	-2.082362	-1.912303	-2.341926
43	6	0	-1.840838	-3.268798	-2.147760
44	6	0	-0.916272	-3.715287	-1.210696
45	6	0	-0.258423	-2.782397	-0.414501
46	7	0	-2.776739	-1.311190	1.460189
47	6	0	-4.137191	-1.557117	1.166763
48	6	0	-4.431380	-2.591975	0.275940
49	6	0	-5.753942	-2.909676	-0.009928
50	6	0	-6.772327	-2.216982	0.634623
51	6	0	-6.492817	-1.208388	1.550724
52	6	0	-5.169586	-0.875341	1.812928
53	35	0	9.224096	-0.236396	-2.197208
54	35	0	-2.716753	7.772209	-1.021735
55	35	0	-2.858398	-4.534591	-3.121394
56	35	0	-8.578426	-2.666049	0.268521
57	1	0	3.856581	0.391061	2.081023
58	1	0	-0.525219	-1.718322	2.664107
59	1	0	-0.926691	-0.290777	3.610119
60	1	0	1.512856	-1.216563	3.828357
61	1	0	1.371322	0.513955	3.573337
62	1	0	-0.875716	1.903464	2.570060
63	1	0	4.742636	-0.459937	4.103110
64	1	0	5.680763	-2.340697	5.419242
65	1	0	5.577135	-4.653751	4.524525
66	1	0	4.525169	-5.078146	2.316595
67	1	0	3.577189	-3.194880	1.009629
68	1	0	1.220920	2.760969	3.070588
69	1	0	3.466902	3.543910	2.387921
70	1	0	4.138051	3.454978	-0.004362
71	1	0	2.515577	2.661174	-1.709162
72	1	0	0.274977	1.879299	-1.022256
73	1	0	-1.119146	4.184177	2.051708
74	1	0	-1.476014	6.524287	1.351223
75	1	0	-3.364397	5.165176	-2.256990
76	1	0	-3.000071	2.814069	-1.565263
77	1	0	4.307966	-1.120158	-2.307427
78	1	0	6.565395	-0.949304	-3.288854
79	1	0	8.154260	0.183120	0.531764
80	1	0	5.918788	0.017545	1.520677
81	1	0	-1.573644	0.073651	-1.696449
82	1	0	-2.797875	-1.584878	-3.087509
83	1	0	-0.739339	-4.777016	-1.080483
84	1	0	0.438022	-3.113505	0.351244
85	1	0	-3.622295	-3.131701	-0.205962
86	1	0	-5.986397	-3.695676	-0.720010
87	1	0	-7.300654	-0.683536	2.048263
88	1	0	-4.933505	-0.085068	2.518410

5a$_{hetero}$–*exo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.146744	-2.110903	0.420478
2	6	0	-3.699052	-1.914274	1.730928
3	6	0	-4.463791	-2.375645	2.803372
4	6	0	-5.693396	-2.983765	2.573420
5	6	0	-6.124068	-3.169665	1.264796
6	6	0	-5.356775	-2.747356	0.183257
7	7	0	-2.404215	-1.408837	1.981076
8	6	0	-1.984354	-0.311811	1.514681
9	6	0	-0.530113	0.107684	1.605732
10	6	0	-0.657461	1.664526	1.578887
11	7	0	-1.849833	1.867960	0.736744

12	6	0	-2.733707	0.810295	0.808388
13	6	0	0.177052	-0.306797	2.916976
14	8	0	-3.878415	0.796425	0.408898
15	6	0	-2.226643	3.128916	0.216142
16	6	0	-1.829650	4.307035	0.852736
17	6	0	-2.184098	5.542177	0.322206
18	6	0	-2.942954	5.591663	-0.840355
19	6	0	-3.350560	4.427693	-1.482179
20	6	0	-2.988700	3.194404	-0.954900
21	6	0	0.596685	2.389405	1.154007
22	6	0	1.306289	3.106469	2.122309
23	6	0	2.493252	3.760568	1.800821
24	6	0	2.995022	3.688342	0.503792
25	6	0	2.294401	2.974626	-0.468171
26	6	0	1.095972	2.340469	-0.151268
27	35	0	-3.430284	7.274040	-1.562879
28	35	0	-7.781769	-4.034045	0.947137
29	7	0	0.140788	-0.375780	0.362317
30	6	0	-0.609805	-1.007209	-0.686375
31	6	0	-1.313993	-0.247875	-1.622772
32	6	0	-2.094827	-0.869258	-2.593765
33	6	0	-2.144117	-2.257611	-2.637479
34	6	0	-1.408320	-3.034118	-1.747623
35	6	0	-0.647031	-2.402334	-0.771810
36	35	0	-3.275833	-3.108374	-3.893476
37	6	0	1.433313	-0.863074	0.532258
38	6	0	1.908589	-1.425348	1.642654
39	6	0	3.392063	-1.626240	1.514061
40	7	0	3.651447	-1.218540	0.125528
41	6	0	2.502685	-0.733013	-0.488468
42	6	0	1.020579	-1.587047	2.829605
43	6	0	4.124839	-0.764848	2.530396
44	6	0	4.777455	-1.346755	3.614584
45	6	0	5.397775	-0.545026	4.572632
46	6	0	5.366926	0.840292	4.444835
47	6	0	4.708211	1.424147	3.361632
48	6	0	4.082472	0.626284	2.410834
49	6	0	4.938799	-1.276033	-0.440328
50	6	0	5.237028	-0.642078	-1.656132
51	6	0	6.519440	-0.715263	-2.186336
52	6	0	7.512903	-1.411292	-1.509617
53	6	0	7.238454	-2.038788	-0.302489
54	6	0	5.955837	-1.971862	0.227782
55	8	0	2.387721	-0.295574	-1.618419
56	35	0	9.260633	-1.504084	-2.239473
57	1	0	3.658103	-2.681453	1.655534
58	1	0	-0.582492	-0.392741	3.699304
59	1	0	0.857537	0.505856	3.198584
60	1	0	0.370597	-2.461596	2.702350
61	1	0	1.591570	-1.722707	3.752867
62	1	0	-0.897570	1.983967	2.603777
63	1	0	4.806779	-2.430204	3.708761
64	1	0	5.908616	-1.005240	5.412452
65	1	0	5.854779	1.465823	5.185648
66	1	0	4.679935	2.504224	3.256537
67	1	0	3.561780	1.083337	1.569890
68	1	0	0.918823	3.162836	3.137491
69	1	0	3.020211	4.326589	2.562826
70	1	0	3.924020	4.188575	0.248791
71	1	0	2.678557	2.908310	-1.481002
72	1	0	0.568630	1.787149	-0.919242
73	1	0	-1.242186	4.269391	1.763061
74	1	0	-1.874906	6.457554	0.813622
75	1	0	-3.941470	4.482029	-2.389376
76	1	0	-3.306804	2.282517	-1.446079
77	1	0	4.466685	-0.099161	-2.183637
78	1	0	6.742629	-0.224518	-3.127252
79	1	0	8.016519	-2.579418	0.224602
80	1	0	5.762737	-2.466564	1.171770
81	1	0	-1.265896	0.835498	-1.586315
82	1	0	-2.660168	-0.278989	-3.306243
83	1	0	-1.455806	-4.116048	-1.797708
84	1	0	-0.091940	-2.994412	-0.049817
85	1	0	-4.093945	-2.249353	3.815638

86	1	0	-6.302053	-3.327066	3.402247
87	1	0	-5.697100	-2.911263	-0.833389
88	1	0	-3.539436	-1.765422	-0.409803

5a$_{hetero}$–*exo′*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.662398	-0.711960	0.208299
2	7	0	0.311304	-0.689119	-0.131234
3	6	0	2.204291	-1.257645	1.305172
4	6	0	3.706508	-1.172081	1.241255
5	7	0	3.936895	-0.511965	-0.044493
6	6	0	2.748422	-0.248980	-0.708022
7	8	0	2.621522	0.246930	-1.811107
8	6	0	5.231676	-0.208687	-0.510667
9	6	0	4.356152	-2.541352	1.333957
10	6	0	-0.149016	0.408116	-0.934467
11	6	0	-0.594014	-1.116790	0.978115
12	6	0	0.036901	-2.295438	1.729532
13	6	0	1.407859	-1.979659	2.335497
14	6	0	-1.950981	-1.510704	0.402732
15	6	0	-2.859108	-0.295401	0.462558
16	7	0	-2.180507	0.647766	1.191354
17	6	0	-0.983978	0.119918	1.866046
18	6	0	-1.255517	-0.184777	3.327440
19	6	0	-2.515511	2.020196	1.245327
20	8	0	-3.956047	-0.178946	-0.046959
21	6	0	4.967024	-2.944691	2.519768
22	6	0	5.510080	-4.223872	2.631463
23	6	0	5.446548	-5.102068	1.553601
24	6	0	4.835433	-4.700544	0.365375
25	6	0	4.287826	-3.426851	0.257057
26	6	0	-2.404514	-0.875300	3.722261
27	6	0	-2.622447	-1.167034	5.065390
28	6	0	-1.700947	-0.762099	6.030122
29	6	0	-0.561487	-0.060354	5.646527
30	6	0	-0.343166	0.227032	4.300850
31	6	0	-1.945763	2.831003	2.231992
32	6	0	-2.159278	4.205739	2.224285
33	6	0	-2.946490	4.768023	1.229567
34	6	0	-3.536390	3.973518	0.252355
35	6	0	-3.327904	2.601365	0.261024
36	6	0	5.476847	0.107698	-1.854822
37	6	0	6.768052	0.398629	-2.279531
38	6	0	7.820719	0.367366	-1.374295
39	6	0	7.598530	0.046012	-0.042146
40	6	0	6.308125	-0.238975	0.386510
41	6	0	0.244518	1.721945	-0.666441
42	6	0	-0.326863	2.783233	-1.356874
43	6	0	-1.302841	2.519330	-2.311141
44	6	0	-1.664928	1.217176	-2.635368
45	6	0	-1.066642	0.160502	-1.954375
46	7	0	-2.197375	-2.691265	0.024365
47	6	0	-3.418967	-3.132576	-0.528291
48	6	0	-3.979922	-4.290231	0.018518
49	6	0	-5.139970	-4.833391	-0.520206
50	6	0	-5.704418	-4.239823	-1.643330
51	6	0	-5.136509	-3.111723	-2.226225
52	6	0	-3.996704	-2.553442	-1.662140
53	35	0	9.579351	0.762370	-1.962721
54	35	0	-3.223688	6.641799	1.201255
55	35	0	-2.201076	3.967174	-3.134061
56	35	0	-7.268807	-4.991172	-2.405545
57	1	0	4.078120	-0.539956	2.059911
58	1	0	0.135792	-3.105835	1.001739
59	1	0	-0.662773	-2.632693	2.497494
60	1	0	1.909326	-2.915020	2.610660
61	1	0	1.316385	-1.394809	3.258546
62	1	0	-0.185898	0.867469	1.800822
63	1	0	5.021705	-2.254210	3.358832
64	1	0	5.986981	-4.528930	3.557543
65	1	0	5.873788	-6.096394	1.635787

66	1	0	4.785617	-5.382000	-0.477965
67	1	0	3.811435	-3.112203	-0.668404
68	1	0	-3.141169	-1.183793	2.983811
69	1	0	-3.517781	-1.705178	5.359399
70	1	0	-1.876426	-0.985581	7.077451
71	1	0	0.154505	0.270218	6.392096
72	1	0	0.542335	0.785314	4.001283
73	1	0	-1.337482	2.400183	3.018856
74	1	0	-1.712191	4.830524	2.989128
75	1	0	-4.140022	4.422789	-0.528022
76	1	0	-3.773285	1.990141	-0.511804
77	1	0	4.661515	0.129803	-2.562516
78	1	0	6.950896	0.643722	-3.319925
79	1	0	8.423506	0.018241	0.660789
80	1	0	6.154337	-0.490414	1.429105
81	1	0	0.991554	1.919666	0.097800
82	1	0	-0.048680	3.806134	-1.128366
83	1	0	-2.406759	1.029893	-3.403934
84	1	0	-1.317181	-0.866351	-2.202232
85	1	0	-3.501631	-4.754566	0.874714
86	1	0	-5.589323	-5.718557	-0.084604
87	1	0	-5.586567	-2.667140	-3.106597
88	1	0	-3.560739	-1.660377	-2.094814

5a$_{homo}$-in/in–*exo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.286054	-1.166597	0.800947
2	7	0	-0.021122	-0.902389	0.400084
3	6	0	1.813015	-0.907307	2.002636
4	6	0	3.315256	-0.982139	1.911512
5	7	0	3.536143	-1.532593	0.573669
6	6	0	2.348117	-1.600842	-0.146060
7	8	0	2.195976	-1.942895	-1.302485
8	6	0	4.824678	-1.847206	0.100679
9	6	0	3.859143	0.433133	2.081706
10	6	0	-0.766688	-1.980759	-0.179343
11	6	0	-0.716282	-0.011625	1.381818
12	6	0	-0.474742	-0.471176	2.823989
13	6	0	1.017716	-0.479835	3.187326
14	6	0	-2.183532	0.043233	1.018827
15	6	0	-2.341296	1.106914	-0.053732
16	7	0	-1.167667	1.820866	-0.055717
17	6	0	-0.252954	1.439747	1.034423
18	6	0	-0.290439	2.424648	2.187986
19	6	0	-0.833312	2.855557	-0.959398
20	8	0	-3.300770	1.238727	-0.787458
21	6	0	4.155926	0.906285	3.360111
22	6	0	4.528274	2.236783	3.548998
23	6	0	4.614336	3.099569	2.458444
24	6	0	4.327793	2.626442	1.177817
25	6	0	3.945335	1.300610	0.989859
26	6	0	-1.497508	2.914838	2.690400
27	6	0	-1.504169	3.792044	3.771672
28	6	0	-0.304064	4.195732	4.354820
29	6	0	0.904253	3.722478	3.849184
30	6	0	0.908689	2.843116	2.769498
31	6	0	0.309010	3.633471	-0.725102
32	6	0	0.678051	4.634748	-1.615125
33	6	0	-0.093990	4.866275	-2.744888
34	6	0	-1.229390	4.105748	-2.993564
35	6	0	-1.601880	3.102679	-2.107243
36	6	0	5.032332	-2.358361	-1.189882
37	6	0	6.317335	-2.665505	-1.620882
38	6	0	7.401249	-2.467261	-0.775452
39	6	0	7.214813	-1.964398	0.504621
40	6	0	5.931809	-1.655817	0.940015
41	6	0	-1.522415	-1.732565	-1.325598
42	6	0	-2.382623	-2.703779	-1.821801
43	6	0	-2.457713	-3.931143	-1.170495
44	6	0	-1.665801	-4.218974	-0.064986
45	6	0	-0.816984	-3.233085	0.430518

46	7	0	-3.039881	-0.753691	1.494499
47	6	0	-4.401690	-0.722831	1.118021
48	6	0	-4.941759	-1.872983	0.537221
49	6	0	-6.287388	-1.911887	0.191181
50	6	0	-7.092434	-0.813882	0.472125
51	6	0	-6.575666	0.323140	1.084151
52	6	0	-5.224202	0.368436	1.402641
53	35	0	9.151123	-2.884914	-1.373882
54	35	0	0.406282	6.233851	-3.956416
55	35	0	-3.728829	-5.205823	-1.757149
56	35	0	-8.934940	-0.871349	0.026292
57	1	0	3.737849	-1.648665	2.673395
58	1	0	-0.897296	-1.478393	2.902321
59	1	0	-1.036084	0.165245	3.512935
60	1	0	1.193060	-1.168883	4.022707
61	1	0	1.346429	0.506390	3.534136
62	1	0	0.765728	1.388491	0.636896
63	1	0	4.090538	0.233763	4.212720
64	1	0	4.755464	2.595608	4.547995
65	1	0	4.908343	4.134090	2.603847
66	1	0	4.399023	3.290993	0.322336
67	1	0	3.719680	0.937554	-0.009784
68	1	0	-2.440569	2.624681	2.232650
69	1	0	-2.448373	4.165901	4.154409
70	1	0	-0.312307	4.883751	5.194109
71	1	0	1.846981	4.038925	4.285258
72	1	0	1.855772	2.482121	2.369847
73	1	0	0.919052	3.482869	0.156865
74	1	0	1.561963	5.232177	-1.422676
75	1	0	-1.825980	4.289902	-3.880046
76	1	0	-2.485493	2.515594	-2.307186
77	1	0	4.192492	-2.513969	-1.850596
78	1	0	6.470033	-3.060593	-2.619170
79	1	0	8.062569	-1.809938	1.162589
80	1	0	5.810623	-1.255666	1.939494
81	1	0	-1.447544	-0.766368	-1.815410
82	1	0	-2.999208	-2.506759	-2.691337
83	1	0	-1.734422	-5.186306	0.419727
84	1	0	-0.213429	-3.427821	1.312713
85	1	0	-4.301181	-2.726405	0.337730
86	1	0	-6.705321	-2.793307	-0.282627
87	1	0	-7.220772	1.166739	1.302401
88	1	0	-4.804447	1.250490	1.876414

4f–R

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.028729	-2.318723	-0.773690
2	6	0	-1.241032	-1.498891	-0.919675
3	7	0	-0.821800	-0.162180	-0.474704
4	6	0	0.524835	-0.028860	-0.237981
5	6	0	1.138932	-1.404033	-0.450698
6	6	0	-1.753621	0.904389	-0.385300
7	6	0	-1.585267	1.936717	0.537190
8	6	0	-2.513081	2.973267	0.618493
9	6	0	-3.630580	2.979587	-0.216801
10	6	0	-3.809285	1.936158	-1.131234
11	6	0	-2.882485	0.911741	-1.215414
12	6	0	-2.403932	-2.049330	-0.121429
13	6	0	-3.413282	-2.760422	-0.767016
14	6	0	-4.459553	-3.319899	-0.034269
15	6	0	-4.503180	-3.160344	1.347348
16	6	0	-3.496891	-2.443090	1.995711
17	6	0	-2.450003	-1.892570	1.265322
18	8	0	1.092676	0.984808	0.123601
19	7	0	2.339614	-1.799876	-0.304304
20	6	0	3.446372	-0.961648	-0.081697
21	6	0	3.698758	0.201128	-0.812176
22	6	0	4.868036	0.929368	-0.615693
23	6	0	5.799895	0.503336	0.334486
24	6	0	5.563722	-0.671687	1.058465
25	6	0	4.414850	-1.407700	0.830053

26	8	0	-4.591039	3.939658	-0.213385
27	8	0	6.963103	1.147460	0.611304
28	6	0	0.124942	-3.639060	-0.904222
29	1	0	-3.529873	-2.312746	3.072839
30	1	0	-4.686120	1.947633	-1.769777
31	1	0	-1.523394	-1.459230	-1.980400
32	1	0	2.979091	0.535085	-1.551242
33	1	0	-0.723790	1.938800	1.191057
34	1	0	5.037716	1.822577	-1.204811
35	1	0	4.238198	-2.334509	1.366750
36	1	0	-3.383829	-2.874373	-1.848482
37	1	0	-1.666663	-1.330456	1.768046
38	1	0	-2.351432	3.761647	1.343678
39	1	0	6.306904	-0.995956	1.779272
40	1	0	-3.045567	0.112953	-1.930852
41	1	0	-5.320207	-3.588591	1.919369
42	1	0	-5.242054	-3.871525	-0.545780
43	1	0	1.087439	-4.125762	-0.782632
44	1	0	-0.742577	-4.255267	-1.120915
45	6	0	7.232804	2.340859	-0.098765
46	1	0	8.190951	2.703539	0.271893
47	1	0	7.305451	2.153352	-1.176117
48	1	0	6.459632	3.095027	0.086370
49	6	0	-4.444025	5.003232	0.708064
50	1	0	-5.301799	5.657087	0.554746
51	1	0	-4.444532	4.635686	1.740489
52	1	0	-3.520120	5.562837	0.522964

4f–S

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.011206	-2.138051	-1.219785
2	6	0	1.320288	-1.452152	-0.971265
3	7	0	0.915558	-0.157644	-0.397483
4	6	0	-0.435828	0.064095	-0.348516
5	6	0	-1.098988	-1.221171	-0.826632
6	6	0	1.859715	0.894597	-0.211584
7	6	0	1.766422	2.047965	-0.984909
8	6	0	2.682593	3.085696	-0.831467
9	6	0	3.714221	2.960079	0.101866
10	6	0	3.809011	1.800943	0.880836
11	6	0	2.885179	0.779275	0.733000
12	6	0	2.249527	-2.235696	-0.067222
13	6	0	3.540983	-2.545637	-0.483440
14	6	0	4.406262	-3.241283	0.362161
15	6	0	3.980746	-3.622876	1.629973
16	6	0	2.684576	-3.315719	2.051008
17	6	0	1.822657	-2.629783	1.204595
18	8	0	-0.971600	1.110555	-0.037225
19	7	0	-2.329732	-1.507384	-0.981800
20	6	0	-3.408017	-0.720197	-0.541961
21	6	0	-3.473076	-0.109692	0.712408
22	6	0	-4.617830	0.568918	1.118749
23	6	0	-5.715742	0.656296	0.258491
24	6	0	-5.666812	0.031727	-0.993899
25	6	0	-4.537197	-0.670172	-1.373733
26	8	0	4.663052	3.903419	0.326658
27	8	0	-6.871871	1.304169	0.553705
28	6	0	-0.175317	-3.372555	-1.688758
29	1	0	2.348859	-3.613687	3.039341
30	1	0	4.611766	1.728621	1.606839
31	1	0	1.834457	-1.259594	-1.922295
32	1	0	-2.625153	-0.174973	1.384684
33	1	0	0.962392	2.140520	-1.707583
34	1	0	-4.639497	1.023977	2.101673
35	1	0	-4.501206	-1.181329	-2.330629
36	1	0	3.876690	-2.232449	-1.468822
37	1	0	0.814296	-2.385303	1.531460
38	1	0	2.582681	3.974430	-1.442574
39	1	0	-6.535884	0.095041	-1.640195
40	1	0	2.952310	-0.106538	1.355334
41	1	0	4.653710	-4.158569	2.292043

42	1	0	5.412573	-3.476203	0.030035
43	1	0	-1.175481	-3.768764	-1.833632
44	1	0	0.672197	-4.006749	-1.931373
45	6	0	4.594080	5.094418	-0.434951
46	1	0	5.428500	5.712277	-0.105381
47	1	0	4.694502	4.885639	-1.505992
48	1	0	3.652470	5.625104	-0.255047
49	6	0	-6.957373	1.946687	1.811295
50	1	0	-7.943353	2.408602	1.848473
51	1	0	-6.860370	1.226480	2.631640
52	1	0	-6.187118	2.719251	1.914319

RCf_{homo}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.799699	0.223616	2.865468
2	6	0	-1.686193	-0.080264	2.072633
3	6	0	-1.620039	-1.354994	1.482672
4	6	0	-2.627319	-2.277005	1.693088
5	6	0	-3.723626	-1.967700	2.507887
6	6	0	-3.796478	-0.712961	3.118210
7	7	0	-0.801592	0.984799	1.839294
8	6	0	0.450961	0.942422	1.598736
9	6	0	1.237590	2.154812	1.320194
10	6	0	2.628762	1.734020	0.891107
11	7	0	2.650007	0.299432	1.206149
12	6	0	1.435879	-0.214133	1.593412
13	6	0	0.798540	3.405840	1.437271
14	6	0	-0.715273	3.454419	-1.296720
15	6	0	-1.187294	2.211885	-1.226224
16	6	0	-0.424027	0.991775	-1.528249
17	6	0	-1.422327	-0.152687	-1.521430
18	7	0	-2.634561	0.375348	-1.144347
19	6	0	-2.599178	1.814265	-0.848162
20	6	0	-3.789527	-0.389154	-0.834160
21	6	0	-3.944469	-1.710204	-1.267445
22	6	0	-5.032477	-2.471204	-0.848019
23	6	0	-5.997070	-1.917651	-0.006743
24	6	0	-5.886356	-0.576665	0.363655
25	6	0	-4.794975	0.175718	-0.036799
26	8	0	-7.065194	-2.594475	0.494595
27	6	0	-7.050608	-4.003028	0.357095
28	8	0	-1.198867	-1.313125	-1.821231
29	7	0	0.822519	1.021141	-1.797382
30	6	0	1.688130	-0.048302	-2.077253
31	6	0	1.656190	-1.313592	-1.481136
32	6	0	2.643646	-2.256864	-1.747819
33	6	0	3.679169	-1.951853	-2.633590
34	6	0	3.721032	-0.691519	-3.242970
35	6	0	2.757764	0.252507	-2.940304
36	6	0	-3.648815	2.607375	-1.599553
37	6	0	-4.243174	3.711312	-0.989254
38	6	0	-5.161622	4.493258	-1.687737
39	6	0	-5.496435	4.167544	-2.999176
40	6	0	-4.908338	3.059947	-3.609918
41	6	0	-3.985849	2.284829	-2.914821
42	8	0	4.699695	-2.793988	-2.939066
43	6	0	4.668283	-4.093868	-2.374619
44	6	0	3.731741	2.509119	1.579222
45	6	0	4.352438	3.564037	0.912114
46	6	0	5.327624	4.327037	1.552908
47	6	0	5.692376	4.030219	2.862938
48	6	0	5.077440	2.971060	3.531129
49	6	0	4.098861	2.216036	2.893833
50	6	0	3.783667	-0.492643	0.890744
51	6	0	4.710569	-0.026412	-0.041538
52	6	0	5.782008	-0.816966	-0.446849
53	6	0	5.938943	-2.096007	0.082991
54	6	0	5.044874	-2.544906	1.060516
55	6	0	3.982185	-1.755681	1.468809
56	8	0	1.209663	-1.372355	1.898746
57	8	0	6.913869	-2.969395	-0.285914

58	6	0	7.732019	-2.595074	-1.379836
59	8	0	-4.666895	-2.937148	2.624831
60	6	0	-5.822238	-2.630863	3.382358
61	1	0	2.711030	1.863228	-0.197511
62	1	0	-1.341265	4.317582	-1.090007
63	1	0	0.319663	3.620971	-1.578269
64	1	0	-0.225477	3.590185	1.746581
65	1	0	1.442041	4.258270	1.239629
66	1	0	-2.730513	1.955397	0.234164
67	1	0	4.074631	3.785905	-0.116283
68	1	0	5.806066	5.145838	1.024683
69	1	0	6.456449	4.617865	3.362014
70	1	0	5.362299	2.733280	4.551303
71	1	0	3.620548	1.388562	3.411754
72	1	0	-3.989871	3.955967	0.040409
73	1	0	-5.619909	5.349941	-1.203509
74	1	0	-6.216771	4.770319	-3.543155
75	1	0	-5.170194	2.799308	-4.630677
76	1	0	-3.529333	1.419600	-3.388684
77	1	0	-4.728532	1.202723	0.299568
78	1	0	-6.655447	-0.140998	0.993801
79	1	0	-5.103195	-3.501433	-1.176652
80	1	0	-3.196587	-2.160328	-1.902586
81	1	0	3.290714	-2.125326	2.211696
82	1	0	5.196071	-3.531449	1.487478
83	1	0	6.460601	-0.432345	-1.198818
84	1	0	4.596334	0.950999	-0.494779
85	1	0	-0.796261	-1.612025	0.831203
86	1	0	-2.602869	-3.246727	1.207160
87	1	0	-4.638241	-0.440123	3.743459
88	1	0	-2.867483	1.219216	3.293963
89	1	0	2.803093	1.246089	-3.376214
90	1	0	4.540888	-0.466065	-3.917354
91	1	0	2.607060	-3.211735	-1.237187
92	1	0	0.871368	-1.562138	-0.778652
93	1	0	8.386380	-3.445136	-1.572465
94	1	0	7.120361	-2.386593	-2.265106
95	1	0	8.341645	-1.716941	-1.137488
96	1	0	5.555859	-4.604828	-2.748082
97	1	0	4.706608	-4.050850	-1.280852
98	1	0	3.770030	-4.635024	-2.692225
99	1	0	-6.461293	-3.512329	3.329638
100	1	0	-5.564664	-2.426025	4.427784
101	1	0	-6.353187	-1.772920	2.955756
102	1	0	-7.905599	-4.372299	0.923729
103	1	0	-7.156184	-4.304774	-0.691105
104	1	0	-6.123362	-4.419096	0.768201

RCf_{hetero}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.566152	-1.444961	3.273925
2	6	0	-1.110417	-0.781182	2.170899
3	6	0	-2.335409	-1.235084	1.654422
4	6	0	-2.953139	-2.361079	2.165836
5	6	0	-2.385001	-3.034969	3.253941
6	6	0	-1.197285	-2.559482	3.817843
7	7	0	-0.605007	0.404859	1.613354
8	6	0	0.620775	0.691900	1.406760
9	6	0	1.054647	1.994680	0.888802
10	6	0	2.471321	1.848424	0.371762
11	7	0	2.858648	0.501685	0.816164
12	6	0	1.858190	-0.186054	1.466380
13	6	0	0.337849	3.116290	0.924004
14	8	0	1.933816	-1.304885	1.940352
15	6	0	4.070184	-0.076837	0.357908
16	6	0	4.844111	0.605660	-0.594786
17	6	0	5.995423	0.036939	-1.110761
18	6	0	6.413625	-1.226614	-0.687624
19	6	0	5.669548	-1.900531	0.278808
20	6	0	4.512647	-1.327520	0.802065
21	6	0	3.394888	2.940385	0.871058

22	6	0	3.610787	4.067011	0.077485
23	6	0	4.400820	5.116459	0.543132
24	6	0	4.987833	5.038258	1.803255
25	6	0	4.779892	3.909687	2.595651
26	6	0	3.983865	2.866145	2.133531
27	8	0	7.541797	-1.714718	-1.275555
28	8	0	-3.065376	-4.120095	3.701408
29	7	0	0.436049	0.748147	-2.000234
30	6	0	1.224802	-0.412814	-1.966392
31	6	0	1.035310	-1.508844	-1.104371
32	6	0	1.944002	-2.549199	-1.092818
33	6	0	3.046331	-2.549170	-1.960372
34	6	0	3.253286	-1.465680	-2.814780
35	6	0	2.363843	-0.395744	-2.778657
36	8	0	3.859475	-3.631731	-1.883200
37	6	0	-0.825202	0.835695	-1.831190
38	6	0	-1.531577	2.125265	-1.841303
39	6	0	-3.021460	1.867870	-1.725095
40	7	0	-3.097813	0.404443	-1.578857
41	6	0	-1.886583	-0.240294	-1.706113
42	6	0	-0.954891	3.322500	-1.924913
43	6	0	-3.665584	2.628289	-0.582777
44	6	0	-4.566476	3.658345	-0.843750
45	6	0	-5.124517	4.389203	0.205071
46	6	0	-4.784470	4.086982	1.520151
47	6	0	-3.877846	3.059000	1.783461
48	6	0	-3.316456	2.334712	0.737096
49	6	0	-4.352357	-0.257490	-1.514875
50	6	0	-4.461727	-1.588013	-1.071598
51	6	0	-5.701787	-2.197238	-0.991198
52	6	0	-6.867059	-1.509212	-1.345680
53	6	0	-6.767616	-0.191497	-1.787583
54	6	0	-5.518520	0.422118	-1.868893
55	8	0	-1.720541	-1.444765	-1.759542
56	8	0	-8.030462	-2.199344	-1.226919
57	1	0	-3.510550	2.154513	-2.665791
58	1	0	0.741386	4.061580	0.572095
59	1	0	-0.674581	3.106052	1.316867
60	1	0	0.124735	3.392967	-2.015783
61	1	0	-1.535224	4.240406	-1.902756
62	1	0	2.442595	1.860513	-0.727316
63	1	0	-4.837401	3.890461	-1.871946
64	1	0	-5.827081	5.188763	-0.008156
65	1	0	-5.221366	4.650554	2.338602
66	1	0	-3.603273	2.822841	2.807188
67	1	0	-2.580226	1.559658	0.942310
68	1	0	3.162175	4.118761	-0.912915
69	1	0	4.563458	5.988738	-0.082188
70	1	0	5.609612	5.850701	2.165830
71	1	0	5.240242	3.842088	3.576448
72	1	0	3.823435	1.984818	2.748939
73	1	0	4.552706	1.584869	-0.952887
74	1	0	6.587396	0.562414	-1.852850
75	1	0	5.967314	-2.879922	0.634170
76	1	0	3.942599	-1.869948	1.540189
77	1	0	-3.575831	-2.146515	-0.804815
78	1	0	-5.788420	-3.224203	-0.651093
79	1	0	-7.646278	0.375607	-2.070017
80	1	0	-5.479287	1.449241	-2.209369
81	1	0	0.190562	-1.529023	-0.425219
82	1	0	1.825542	-3.379831	-0.405108
83	1	0	4.114630	-1.421836	-3.470375
84	1	0	2.533363	0.473631	-3.407330
85	1	0	-2.794515	-0.686089	0.838003
86	1	0	-3.890596	-2.722770	1.754730
87	1	0	-0.753221	-3.047030	4.677389
88	1	0	0.353876	-1.083726	3.715790
89	6	0	-2.519035	-4.828629	4.797525
90	1	0	-3.197129	-5.659647	4.988364
91	1	0	-1.522126	-5.216598	4.560280
92	1	0	-2.458987	-4.194214	5.689085
93	6	0	-9.223121	-1.526353	-1.580893
94	1	0	-10.032064	-2.237771	-1.418795
95	1	0	-9.381390	-0.643349	-0.951258

96	1	0	-9.209018	-1.222824	-2.633964
97	6	0	8.047307	-2.941152	-0.783879
98	1	0	8.961214	-3.138823	-1.343146
99	1	0	8.277606	-2.872442	0.285313
100	1	0	7.336672	-3.760017	-0.946677
101	6	0	4.952379	-3.689871	-2.779205
102	1	0	5.446043	-4.643703	-2.591408
103	1	0	4.610427	-3.657069	-3.820153
104	1	0	5.658291	-2.869283	-2.603228

RCf_{homo}–*exo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.736232	-2.643454	1.188811
2	6	0	-3.422702	-2.992966	0.874029
3	6	0	-3.197431	-3.865339	-0.201069
4	6	0	-4.249132	-4.306995	-0.986177
5	6	0	-5.561933	-3.934514	-0.675383
6	6	0	-5.803484	-3.112624	0.428279
7	7	0	-2.306660	-2.617896	1.647644
8	6	0	-2.037600	-1.419966	1.981744
9	6	0	-0.872708	-1.054712	2.805984
10	6	0	-0.788333	0.462750	2.878348
11	7	0	-1.886495	0.894235	2.007016
12	6	0	-2.704332	-0.121795	1.567597
13	6	0	-0.056985	-1.925371	3.394281
14	8	0	-3.745765	0.011753	0.955097
15	6	0	-2.161174	2.267051	1.777879
16	6	0	-1.745962	3.236793	2.698527
17	6	0	-1.977045	4.579975	2.450240
18	6	0	-2.623602	4.984091	1.277306
19	6	0	-3.030813	4.021155	0.352792
20	6	0	-2.795686	2.672059	0.603638
21	6	0	0.568896	1.017973	2.483866
22	6	0	1.587280	1.047980	3.439292
23	6	0	2.857665	1.513031	3.105685
24	6	0	3.115958	1.971836	1.814817
25	6	0	2.097852	1.961907	0.862598
26	6	0	0.830574	1.486330	1.195673
27	8	0	-2.800544	6.322881	1.124641
28	8	0	-6.529637	-4.429476	-1.491802
29	7	0	-0.509870	-0.829905	-0.893742
30	6	0	-1.317638	0.070728	-1.603853
31	6	0	-0.976699	1.372519	-2.025643
32	6	0	-1.915607	2.178335	-2.642644
33	6	0	-3.220972	1.718174	-2.862221
34	6	0	-3.580124	0.433991	-2.444385
35	6	0	-2.635766	-0.360407	-1.803694
36	8	0	-4.063761	2.595342	-3.462127
37	6	0	0.762072	-0.894412	-0.815464
38	6	0	1.443310	-1.864893	0.060240
39	6	0	2.879902	-1.413272	0.221755
40	7	0	3.054490	-0.508848	-0.922601
41	6	0	1.875264	-0.126910	-1.515802
42	6	0	0.901301	-2.954050	0.597292
43	6	0	3.876911	-2.547501	0.256888
44	6	0	4.387835	-2.974244	1.481314
45	6	0	5.261265	-4.059425	1.540882
46	6	0	5.634231	-4.715131	0.371209
47	6	0	5.128255	-4.286886	-0.856712
48	6	0	4.249382	-3.210847	-0.913709
49	6	0	4.303579	0.103741	-1.193222
50	6	0	4.626932	0.553478	-2.482126
51	6	0	5.854056	1.147202	-2.722484
52	6	0	6.792181	1.296050	-1.695021
53	6	0	6.483895	0.834356	-0.415531
54	6	0	5.245374	0.242375	-0.173934
55	8	0	1.775357	0.658204	-2.443304
56	8	0	7.965125	1.888454	-2.038853
57	1	0	2.958259	-0.829759	1.153671
58	1	0	-0.242692	-2.989502	3.283904
59	1	0	0.802985	-1.613788	3.979181

60	1	0	-0.151987	-3.169700	0.447594
61	1	0	1.488618	-3.634320	1.207628
62	1	0	-1.001706	0.778342	3.909421
63	1	0	4.101469	-2.450954	2.391695
64	1	0	5.653887	-4.385459	2.498965
65	1	0	6.319690	-5.555732	0.413218
66	1	0	5.419767	-4.793920	-1.771219
67	1	0	3.853124	-2.873839	-1.868295
68	1	0	1.382653	0.719418	4.455795
69	1	0	3.638998	1.533462	3.859151
70	1	0	4.100759	2.345647	1.552342
71	1	0	2.290598	2.322711	-0.145015
72	1	0	0.029404	1.502130	0.462354
73	1	0	-1.228210	2.949692	3.607843
74	1	0	-1.655791	5.339294	3.155198
75	1	0	-3.518926	4.297205	-0.575172
76	1	0	-3.105954	1.932164	-0.122672
77	1	0	3.913205	0.440955	-3.286446
78	1	0	6.113228	1.500138	-3.715135
79	1	0	7.190909	0.922498	0.400546
80	1	0	5.024512	-0.111471	0.827244
81	1	0	0.022460	1.753586	-1.869106
82	1	0	-1.663646	3.186850	-2.954319
83	1	0	-4.586828	0.056843	-2.577665
84	1	0	-2.916749	-1.340505	-1.429343
85	1	0	-2.180432	-4.170510	-0.428224
86	1	0	-4.080778	-4.958657	-1.837114
87	1	0	-6.811441	-2.824394	0.701845
88	1	0	-4.925677	-1.994910	2.036609
89	6	0	-7.867063	-4.067679	-1.208945
90	1	0	-8.478890	-4.548568	-1.971486
91	1	0	-8.173380	-4.422565	-0.218227
92	1	0	-8.003515	-2.981478	-1.261876
93	6	0	-3.423022	6.761508	-0.067548
94	1	0	-3.464349	7.848428	-0.005652
95	1	0	-2.842394	6.466980	-0.949214
96	1	0	-4.439602	6.361316	-0.154444
97	6	0	8.932230	2.054623	-1.020314
98	1	0	9.784527	2.545493	-1.488767
99	1	0	8.548739	2.683854	-0.208922
100	1	0	9.247096	1.087845	-0.611121
101	6	0	-5.400241	2.176511	-3.670949
102	1	0	-5.906146	3.011055	-4.154986
103	1	0	-5.441053	1.296312	-4.321940
104	1	0	-5.894669	1.948655	-2.720106

RCf$_{hetero}$–*exo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.446314	-2.260833	-0.533290
2	6	0	4.673573	-1.286023	-1.160660
3	6	0	5.314897	-0.206742	-1.786333
4	6	0	6.696688	-0.131240	-1.793876
5	6	0	7.471265	-1.116203	-1.170615
6	6	0	6.837917	-2.183211	-0.534242
7	7	0	3.258082	-1.364073	-1.121641
8	6	0	2.562723	-2.103698	-0.059751
9	6	0	1.086426	-1.901336	-0.390115
10	6	0	1.012576	-1.210539	-1.691334
11	6	0	2.432215	-0.871177	-2.097111
12	7	0	0.059543	-0.857104	-2.453651
13	6	0	-1.271686	-1.274544	-2.208557
14	6	0	-2.244417	-0.371195	-1.763699
15	6	0	-3.571203	-0.764094	-1.652597
16	6	0	-3.960143	-2.054983	-2.026567
17	6	0	-2.990879	-2.968793	-2.445214
18	6	0	-1.656298	-2.575893	-2.529660
19	8	0	-5.295299	-2.324584	-1.977061
20	6	0	0.080536	-2.247647	0.413310
21	6	0	2.963939	-1.654378	1.332204
22	6	0	2.928128	-2.571151	2.384009
23	6	0	3.302307	-2.185297	3.670087

24	6	0	3.742850	-0.884772	3.905974
25	6	0	3.782352	0.031943	2.855920
26	6	0	3.379925	-0.345158	1.577910
27	8	0	2.759150	-0.289908	-3.114160
28	8	0	8.817034	-0.943685	-1.231377
29	6	0	0.269734	-0.168512	3.127800
30	6	0	-0.582485	0.583660	2.435266
31	6	0	-1.904624	0.148625	1.949674
32	6	0	-2.503759	1.329918	1.203291
33	7	0	-1.571387	2.335559	1.250058
34	6	0	-0.356241	2.022471	2.016793
35	7	0	-2.307653	-1.050437	2.111018
36	6	0	-3.515108	-1.623879	1.700717
37	6	0	-4.760566	-0.986394	1.660356
38	6	0	-5.894990	-1.672134	1.245498
39	6	0	-5.799426	-3.011517	0.857474
40	6	0	-4.572445	-3.677308	0.951213
41	6	0	-3.454255	-2.993375	1.391117
42	8	0	-6.841353	-3.744688	0.392556
43	6	0	0.897826	2.244002	1.193719
44	6	0	1.996963	2.899593	1.743412
45	6	0	3.135211	3.136195	0.971626
46	6	0	3.170450	2.729625	-0.359730
47	6	0	2.072560	2.066807	-0.913697
48	6	0	0.948001	1.815208	-0.134037
49	6	0	-1.735759	3.604816	0.635110
50	6	0	-1.109073	4.728264	1.190763
51	6	0	-1.230316	5.969957	0.592126
52	6	0	-1.981037	6.121753	-0.578393
53	6	0	-2.603185	5.006814	-1.140344
54	6	0	-2.474692	3.756665	-0.538389
55	8	0	-3.580854	1.394454	0.634690
56	8	0	-2.041491	7.378500	-1.088617
57	1	0	2.793998	-3.173503	-0.158716
58	1	0	-0.000757	-1.187312	3.388127
59	1	0	1.241313	0.200209	3.440322
60	1	0	-0.955321	-2.097027	0.135401
61	1	0	0.274184	-2.682512	1.390916
62	1	0	-0.312622	2.658298	2.910197
63	1	0	2.621977	-3.597883	2.193982
64	1	0	3.270513	-2.906905	4.480424
65	1	0	4.056987	-0.588519	4.902029
66	1	0	4.120998	1.049496	3.028301
67	1	0	3.409870	0.374551	0.764649
68	1	0	1.958637	3.241554	2.775631
69	1	0	3.984654	3.653539	1.407130
70	1	0	4.047348	2.931414	-0.967346
71	1	0	2.089646	1.748558	-1.951581
72	1	0	0.089138	1.306208	-0.566370
73	1	0	-0.517082	4.637842	2.094926
74	1	0	-0.745517	6.842438	1.016883
75	1	0	-3.184770	5.088913	-2.050602
76	1	0	-2.964265	2.901449	-0.984308
77	1	0	4.726439	0.560121	-2.272023
78	1	0	7.203744	0.697230	-2.277197
79	1	0	7.406110	-2.957551	-0.033452
80	1	0	4.974291	-3.092671	-0.021663
81	1	0	-1.960588	0.648881	-1.517892
82	1	0	-4.319867	-0.072359	-1.282366
83	1	0	-3.257449	-3.981965	-2.721528
84	1	0	-0.905074	-3.280621	-2.873723
85	1	0	-2.499705	-3.502650	1.484675
86	1	0	-4.524510	-4.727779	0.682293
87	1	0	-6.844032	-1.150476	1.216599
88	1	0	-4.842844	0.051741	1.951505
89	6	0	9.626515	-1.922792	-0.609215
90	1	0	10.657588	-1.609829	-0.769537
91	1	0	9.424603	-1.978329	0.466617
92	1	0	9.470183	-2.910055	-1.058724
93	6	0	-8.043890	-3.053078	0.109521
94	1	0	-8.710301	-3.781232	-0.352776
95	1	0	-8.507337	-2.667530	1.024339
96	1	0	-7.858781	-2.224694	-0.584358
97	6	0	-5.705762	-3.599122	-2.429599

98	1	0	-6.794230	-3.607708	-2.376546
99	1	0	-5.387733	-3.769537	-3.464997
100	1	0	-5.309903	-4.394168	-1.787005
101	6	0	-2.770443	7.559058	-2.287928
102	1	0	-2.692223	8.617654	-2.532936
103	1	0	-2.345264	6.962517	-3.102923
104	1	0	-3.824863	7.291733	-2.154724

TSf_{homo}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.096823	-1.768524	-1.096882
2	6	0	-3.949165	-0.414377	-0.774373
3	6	0	-5.006007	0.230113	-0.113957
4	6	0	-6.139802	-0.471149	0.263306
5	6	0	-6.254347	-1.835256	-0.009736
6	6	0	-5.235080	-2.472449	-0.713999
7	7	0	-2.756943	0.301878	-1.054308
8	6	0	-2.639575	1.723458	-0.706932
9	6	0	-1.190851	2.018897	-0.987271
10	6	0	-0.524458	0.830109	-1.404089
11	6	0	-1.570782	-0.260079	-1.475269
12	7	0	0.751329	0.842147	-1.625087
13	6	0	1.615088	-0.216974	-1.894073
14	6	0	2.798198	0.135317	-2.561499
15	6	0	3.799135	-0.791397	-2.829954
16	6	0	3.657178	-2.099640	-2.364562
17	6	0	2.491076	-2.465822	-1.674504
18	6	0	1.482012	-1.550056	-1.450531
19	8	0	4.584910	-3.076020	-2.526508
20	6	0	5.752387	-2.745542	-3.257259
21	6	0	-0.519964	3.221782	-0.849311
22	6	0	-3.564315	2.620338	-1.512146
23	6	0	-4.083918	3.773017	-0.923366
24	6	0	-4.878747	4.645735	-1.664097
25	6	0	-5.163727	4.364411	-2.997767
26	6	0	-4.649802	3.209819	-3.587213
27	6	0	-3.850177	2.342550	-2.849105
28	8	0	-1.405044	-1.404689	-1.861935
29	8	0	-7.378313	-2.452034	0.450234
30	6	0	-7.417361	-3.862922	0.349416
31	6	0	0.520009	3.222172	0.848100
32	6	0	1.190915	2.019357	0.986568
33	6	0	0.524534	0.830721	1.403829
34	6	0	1.570833	-0.259475	1.475239
35	7	0	2.756985	0.302337	1.054060
36	6	0	2.639648	1.723838	0.706381
37	7	0	-0.751236	0.842864	1.624915
38	6	0	-1.615040	-0.216122	1.894260
39	6	0	-1.482086	-1.549330	1.451066
40	6	0	-2.491228	-2.464950	1.675289
41	6	0	-3.657286	-2.098484	2.365272
42	6	0	-3.799093	-0.790125	2.830387
43	6	0	-2.798089	0.136436	2.561660
44	8	0	1.405076	-1.403982	1.862205
45	6	0	3.949207	-0.413985	0.774299
46	6	0	4.096760	-1.768120	1.096891
47	6	0	5.235053	-2.472101	0.714222
48	6	0	6.254449	-1.834993	0.010075
49	6	0	6.139983	-0.470904	-0.263093
50	6	0	5.006163	0.230422	0.113975
51	6	0	3.564314	2.620872	1.511521
52	6	0	4.084006	3.773434	0.922590
53	6	0	4.878759	4.646275	1.663259
54	6	0	5.163575	4.365192	2.997016
55	6	0	4.649563	3.210715	3.586612
56	6	0	3.850015	2.343325	2.848565
57	8	0	7.378463	-2.451855	-0.449678
58	6	0	7.417444	-3.862734	-0.348688
59	8	0	-4.585111	-3.074729	2.527453
60	6	0	-5.752610	-2.743961	3.258031
61	1	0	-2.846654	1.846529	0.367046

62	1	0	1.095199	4.129038	0.677943
63	1	0	-0.371933	3.328154	1.459500
64	1	0	0.371968	3.327512	-1.460772
65	1	0	-1.095172	4.128709	-0.679543
66	1	0	2.846818	1.846689	-0.367602
67	1	0	-3.870573	3.983796	0.122799
68	1	0	-5.280683	5.539074	-1.196302
69	1	0	-5.788001	5.038815	-3.575313
70	1	0	-4.873327	2.983778	-4.625202
71	1	0	-3.451866	1.440713	-3.306678
72	1	0	3.870798	3.984028	-0.123639
73	1	0	5.280766	5.539522	1.195350
74	1	0	5.787790	5.039693	3.574511
75	1	0	4.872962	2.984856	4.624667
76	1	0	3.451639	1.441578	3.306258
77	1	0	4.946464	1.281887	-0.138312
78	1	0	6.946364	0.026834	-0.792501
79	1	0	5.297608	-3.525731	0.959103
80	1	0	3.308635	-2.285217	1.621588
81	1	0	-3.308806	-2.285673	-1.621690
82	1	0	-5.297718	-3.526090	-0.958816
83	1	0	-6.946100	0.026655	0.792780
84	1	0	-4.946234	1.281593	0.138251
85	1	0	0.589517	-1.855800	-0.921694
86	1	0	2.409052	-3.484175	-1.308300
87	1	0	4.692833	-0.475265	-3.354380
88	1	0	2.910637	1.166027	-2.885798
89	1	0	-2.910423	1.167235	2.885709
90	1	0	-4.692741	-0.473794	3.354781
91	1	0	-2.409311	-3.483397	1.309325
92	1	0	-0.589627	-1.855281	0.922285
93	1	0	-8.323920	-4.180187	0.864684
94	1	0	-7.462351	-4.187128	-0.696566
95	1	0	-6.539527	-4.311042	0.830436
96	1	0	-6.349599	-3.655023	3.302969
97	1	0	-5.500138	-2.422154	4.274788
98	1	0	-6.324808	-1.958982	2.751500
99	1	0	6.349237	-3.656700	-3.302122
100	1	0	5.499860	-2.423864	-4.274043
101	1	0	6.324751	-1.960563	-2.750913
102	1	0	8.324042	-4.180098	-0.863826
103	1	0	7.462310	-4.186811	0.697339
104	1	0	6.539636	-4.310873	-0.829740

TSf_{hetero}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.728722	-0.817762	3.303472
2	6	0	-1.176917	-0.624959	1.993611
3	6	0	-2.197506	-1.458752	1.511748
4	6	0	-2.713937	-2.479875	2.292689
5	6	0	-2.250549	-2.668683	3.597867
6	6	0	-1.258430	-1.824120	4.104622
7	7	0	-0.761689	0.457559	1.197811
8	6	0	0.470726	0.748125	0.976257
9	6	0	0.890213	1.924400	0.265362
10	6	0	2.371789	1.844047	-0.006067
11	7	0	2.759466	0.572631	0.618588
12	6	0	1.719073	-0.069419	1.254516
13	6	0	0.064482	3.022122	0.051139
14	8	0	1.772972	-1.115749	1.872534
15	6	0	4.027988	-0.002526	0.351177
16	6	0	4.929651	0.671300	-0.489069
17	6	0	6.134920	0.091167	-0.845891
18	6	0	6.482357	-1.175047	-0.369175
19	6	0	5.610021	-1.838457	0.490585
20	6	0	4.396758	-1.255713	0.851627
21	6	0	3.128308	3.042980	0.537184
22	6	0	3.388189	4.123201	-0.306668
23	6	0	4.018525	5.265339	0.183618
24	6	0	4.400301	5.328082	1.521342
25	6	0	4.146760	4.247537	2.365615

26	6	0	3.509427	3.110745	1.877311
27	8	0	7.672846	-1.676878	-0.803385
28	8	0	-2.827788	-3.683521	4.296814
29	7	0	0.500667	0.500912	-1.993587
30	6	0	1.289848	-0.647789	-1.942419
31	6	0	1.043615	-1.785870	-1.146329
32	6	0	1.975484	-2.802480	-1.082070
33	6	0	3.163171	-2.738149	-1.828700
34	6	0	3.421613	-1.622583	-2.626129
35	6	0	2.500986	-0.580702	-2.645931
36	8	0	4.001821	-3.794395	-1.696779
37	6	0	-0.795877	0.569702	-1.913816
38	6	0	-1.434181	1.829849	-1.840507
39	6	0	-2.922088	1.649506	-1.694420
40	7	0	-3.069724	0.191768	-1.653272
41	6	0	-1.877398	-0.482687	-1.845585
42	6	0	-0.706591	3.004929	-1.734205
43	6	0	-3.488498	2.396662	-0.500254
44	6	0	-3.854966	3.734327	-0.664810
45	6	0	-4.298911	4.482820	0.423001
46	6	0	-4.392542	3.891603	1.680788
47	6	0	-4.046891	2.550996	1.842302
48	6	0	-3.594715	1.804861	0.757132
49	6	0	-4.353026	-0.411296	-1.616513
50	6	0	-4.520745	-1.782497	-1.352289
51	6	0	-5.790559	-2.331324	-1.292449
52	6	0	-6.927760	-1.542091	-1.488153
53	6	0	-6.770843	-0.181851	-1.746990
54	6	0	-5.493296	0.371881	-1.808214
55	8	0	-1.746612	-1.686756	-1.971464
56	8	0	-8.124171	-2.181332	-1.405851
57	1	0	-3.413236	2.026524	-2.604268
58	1	0	0.544194	3.989993	-0.081973
59	1	0	-0.863270	3.035684	0.619143
60	1	0	0.257612	3.006237	-2.236966
61	1	0	-1.236009	3.954391	-1.714469
62	1	0	2.538913	1.767495	-1.091739
63	1	0	-3.799268	4.191231	-1.650925
64	1	0	-4.579516	5.522272	0.284627
65	1	0	-4.742499	4.470428	2.529785
66	1	0	-4.127121	2.079819	2.817064
67	1	0	-3.322696	0.763652	0.886586
68	1	0	3.100043	4.065360	-1.354931
69	1	0	4.217844	6.100091	-0.481130
70	1	0	4.897846	6.213266	1.904679
71	1	0	4.446879	4.290453	3.407981
72	1	0	3.313329	2.267240	2.534085
73	1	0	4.698100	1.654025	-0.880837
74	1	0	6.825663	0.610722	-1.501802
75	1	0	5.847594	-2.820138	0.883445
76	1	0	3.727228	-1.794716	1.503577
77	1	0	-3.658120	-2.417841	-1.212380
78	1	0	-5.921971	-3.389362	-1.090790
79	1	0	-7.626476	0.464693	-1.899800
80	1	0	-5.409383	1.435737	-1.996059
81	1	0	0.138481	-1.847607	-0.552240
82	1	0	1.813273	-3.665444	-0.444674
83	1	0	4.341443	-1.534402	-3.191530
84	1	0	2.700717	0.310297	-3.234533
85	1	0	-2.567810	-1.312134	0.502553
86	1	0	-3.490941	-3.135299	1.912255
87	1	0	-0.889086	-1.939909	5.116730
88	1	0	0.042063	-0.165216	3.700462
89	6	0	-2.373547	-3.903399	5.617062
90	1	0	-2.943379	-4.750955	5.996831
91	1	0	-1.304548	-4.144918	5.634372
92	1	0	-2.556178	-3.028071	6.251340
93	6	0	-9.289014	-1.403213	-1.599310
94	1	0	-10.131042	-2.086813	-1.496331
95	1	0	-9.366841	-0.611642	-0.845141
96	1	0	-9.303840	-0.953443	-2.598806
97	6	0	8.107449	-2.894792	-0.229694
98	1	0	9.088715	-3.098701	-0.657193
99	1	0	8.190941	-2.809703	0.859717

100	1	0	7.426376	-3.718445	-0.474314
101	6	0	5.175419	-3.796804	-2.487314
102	1	0	5.686288	-4.734055	-2.265877
103	1	0	4.929980	-3.758972	-3.554894
104	1	0	5.828713	-2.952906	-2.235685

TSf$_{homo}$–*exo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.001861	-2.274946	-1.207663
2	6	0	3.770188	-2.798150	-0.795647
3	6	0	3.777122	-3.843494	0.146925
4	6	0	4.958164	-4.293168	0.708928
5	6	0	6.180857	-3.745485	0.302378
6	6	0	6.197465	-2.743797	-0.672191
7	7	0	2.529366	-2.447343	-1.332583
8	6	0	2.151531	-1.248239	-1.631791
9	6	0	0.874958	-0.973155	-2.209558
10	6	0	0.743086	0.507985	-2.468709
11	7	0	1.868425	1.057805	-1.713031
12	6	0	2.787339	0.100979	-1.334666
13	6	0	-0.082260	-1.952571	-2.521573
14	8	0	3.872851	0.322756	-0.833398
15	6	0	2.097479	2.448962	-1.582270
16	6	0	1.648401	3.341174	-2.561486
17	6	0	1.836660	4.704607	-2.401157
18	6	0	2.480145	5.201593	-1.262998
19	6	0	2.924976	4.314018	-0.281338
20	6	0	2.725462	2.945059	-0.440873
21	6	0	-0.618869	1.096552	-2.158729
22	6	0	-1.610385	1.025323	-3.141321
23	6	0	-2.895228	1.501680	-2.888693
24	6	0	-3.194945	2.069383	-1.651414
25	6	0	-2.201925	2.166565	-0.677841
26	6	0	-0.919785	1.683021	-0.930368
27	8	0	2.618981	6.552823	-1.200101
28	8	0	7.290128	-4.257757	0.898033
29	7	0	0.373294	-0.860391	0.774070
30	6	0	1.175654	-0.045748	1.558364
31	6	0	0.852611	1.202630	2.145658
32	6	0	1.798276	1.905978	2.864055
33	6	0	3.098462	1.401876	3.032578
34	6	0	3.442425	0.174541	2.460074
35	6	0	2.490256	-0.519708	1.726418
36	8	0	3.942622	2.175778	3.753497
37	6	0	-0.928812	-0.889985	0.660173
38	6	0	-1.532861	-1.772961	-0.260953
39	6	0	-2.997064	-1.457446	-0.387196
40	7	0	-3.221169	-0.553497	0.741616
41	6	0	-2.057756	-0.149357	1.355672
42	6	0	-0.811725	-2.687465	-1.042485
43	6	0	-3.887260	-2.682050	-0.368821
44	6	0	-4.397668	-3.184993	-1.563963
45	6	0	-5.165453	-4.348837	-1.567142
46	6	0	-5.431830	-5.007932	-0.370561
47	6	0	-4.925307	-4.503957	0.827990
48	6	0	-4.151960	-3.348237	0.828971
49	6	0	-4.498602	-0.002720	1.004844
50	6	0	-4.849000	0.437731	2.289867
51	6	0	-6.106984	0.966466	2.524030
52	6	0	-7.050803	1.055499	1.495210
53	6	0	-6.715216	0.602280	0.219859
54	6	0	-5.444885	0.078996	-0.016286
55	8	0	-1.992151	0.634642	2.287616
56	8	0	-8.255799	1.585461	1.833345
57	1	0	-3.155532	-0.906920	-1.331079
58	1	0	0.351106	-2.890570	-2.865808
59	1	0	-0.936297	-1.627194	-3.113705
60	1	0	0.119080	-3.026829	-0.583381
61	1	0	-1.406359	-3.476143	-1.502337
62	1	0	0.924036	0.672911	-3.545183
63	1	0	-4.196001	-2.660828	-2.496147

64	1	0	-5.560043	-4.733384	-2.502430
65	1	0	-6.035125	-5.910263	-0.368927
66	1	0	-5.133687	-5.013986	1.763264
67	1	0	-3.755700	-2.951043	1.760125
68	1	0	-1.371912	0.603596	-4.115490
69	1	0	-3.655808	1.439096	-3.661046
70	1	0	-4.194361	2.440261	-1.446296
71	1	0	-2.430334	2.597995	0.292799
72	1	0	-0.141687	1.765799	-0.176835
73	1	0	1.140532	2.972786	-3.447613
74	1	0	1.489193	5.407771	-3.150553
75	1	0	3.414386	4.668576	0.618204
76	1	0	3.056598	2.256133	0.327422
77	1	0	-4.131428	0.369885	3.095813
78	1	0	-6.386294	1.312068	3.513874
79	1	0	-7.424224	0.646449	-0.598040
80	1	0	-5.203015	-0.265016	-1.016306
81	1	0	-0.145326	1.605522	2.047850
82	1	0	1.557267	2.865744	3.309677
83	1	0	4.440432	-0.235893	2.554969
84	1	0	2.750661	-1.465516	1.261155
85	1	0	2.825723	-4.276213	0.442087
86	1	0	4.963619	-5.081053	1.454929
87	1	0	7.131534	-2.320198	-1.021866
88	1	0	5.024916	-1.496712	-1.960609
89	6	0	8.541831	-3.725918	0.510573
90	1	0	9.290966	-4.253581	1.100070
91	1	0	8.731782	-3.894128	-0.555676
92	1	0	8.599187	-2.652193	0.722797
93	6	0	3.246469	7.086960	-0.050732
94	1	0	3.258939	8.167875	-0.186855
95	1	0	2.686087	6.839563	0.858122
96	1	0	4.274315	6.719236	0.047171
97	6	0	-9.230134	1.684308	0.813353
98	1	0	-10.110239	2.129007	1.276571
99	1	0	-8.884085	2.326774	-0.004579
100	1	0	-9.487454	0.696674	0.413607
101	6	0	5.272131	1.714919	3.918520
102	1	0	5.782492	2.472786	4.511490
103	1	0	5.294037	0.757262	4.449828
104	1	0	5.772988	1.605654	2.950434

TSf_{hetero}–*exo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.298461	-2.493523	-0.709909
2	6	0	4.482797	-1.477190	-1.209361
3	6	0	5.073562	-0.455224	-1.970887
4	6	0	6.433534	-0.475546	-2.228335
5	6	0	7.245498	-1.499753	-1.730450
6	6	0	6.669170	-2.510867	-0.964104
7	7	0	3.099562	-1.469381	-0.913623
8	6	0	2.544794	-2.288081	0.164260
9	6	0	1.053625	-2.001000	0.098436
10	6	0	0.796746	-1.178294	-1.020962
11	6	0	2.127215	-0.812265	-1.634900
12	7	0	-0.270119	-0.633086	-1.545135
13	6	0	-1.539649	-1.165943	-1.530329
14	6	0	-2.598407	-0.305146	-1.897672
15	6	0	-3.883437	-0.774030	-2.061784
16	6	0	-4.159116	-2.143235	-1.913024
17	6	0	-3.120447	-3.024016	-1.583820
18	6	0	-1.839022	-2.534006	-1.375461
19	8	0	-5.440308	-2.518350	-2.132413
20	6	0	0.183263	-2.259843	1.159502
21	6	0	3.140841	-1.978064	1.522785
22	6	0	3.238403	-2.985708	2.482267
23	6	0	3.697929	-2.694164	3.765658
24	6	0	4.074989	-1.393405	4.089846
25	6	0	3.991537	-0.387828	3.126714
26	6	0	3.523755	-0.676887	1.848182
27	8	0	2.291523	-0.112946	-2.617381

28	8	0	8.567897	-1.420231	-2.038486
29	6	0	-0.027790	-0.764925	2.366734
30	6	0	-0.726157	0.293257	1.785187
31	6	0	-2.090213	0.220174	1.361431
32	6	0	-2.419725	1.558588	0.723543
33	7	0	-1.291117	2.334444	0.842558
34	6	0	-0.239198	1.715878	1.654531
35	7	0	-2.746748	-0.892376	1.504193
36	6	0	-4.046488	-1.254521	1.228591
37	6	0	-5.106869	-0.446157	0.772231
38	6	0	-6.355504	-0.990165	0.505166
39	6	0	-6.576394	-2.361357	0.673499
40	6	0	-5.554918	-3.172553	1.188473
41	6	0	-4.318743	-2.623935	1.454035
42	8	0	-7.729507	-2.994523	0.358793
43	6	0	1.162780	1.984408	1.148321
44	6	0	2.131259	2.425164	2.052793
45	6	0	3.411572	2.757722	1.616023
46	6	0	3.730822	2.651155	0.264086
47	6	0	2.765834	2.212143	-0.641846
48	6	0	1.485212	1.878427	-0.204398
49	6	0	-1.235444	3.696368	0.451386
50	6	0	-0.588419	4.637758	1.260326
51	6	0	-0.512622	5.963717	0.868367
52	6	0	-1.089298	6.379506	-0.336186
53	6	0	-1.734748	5.444920	-1.147158
54	6	0	-1.797042	4.109656	-0.754584
55	8	0	-3.454622	1.921328	0.188146
56	8	0	-0.967092	7.700852	-0.629600
57	1	0	2.716087	-3.351484	-0.061868
58	1	0	-0.635652	-1.411655	2.994915
59	1	0	0.975741	-0.567295	2.739019
60	1	0	-0.881943	-2.333897	0.950065
61	1	0	0.544288	-2.955059	1.914749
62	1	0	-0.289820	2.139761	2.671718
63	1	0	2.954613	-4.004188	2.224254
64	1	0	3.767592	-3.484119	4.506964
65	1	0	4.439143	-1.164583	5.086515
66	1	0	4.288394	0.628085	3.369639
67	1	0	3.453137	0.105896	1.096737
68	1	0	1.875713	2.523921	3.106015
69	1	0	4.153004	3.107529	2.328250
70	1	0	4.725386	2.912259	-0.084427
71	1	0	2.999731	2.125425	-1.697494
72	1	0	0.734312	1.545958	-0.917663
73	1	0	-0.136691	4.335434	2.199430
74	1	0	-0.009506	6.700136	1.485854
75	1	0	-2.183066	5.735068	-2.089679
76	1	0	-2.291846	3.386186	-1.390396
77	1	0	4.459796	0.340525	-2.367461
78	1	0	6.894327	0.309444	-2.819130
79	1	0	7.266075	-3.316880	-0.554586
80	1	0	4.880360	-3.287238	-0.101278
81	1	0	-2.370140	0.744058	-2.055994
82	1	0	-4.698041	-0.107375	-2.324813
83	1	0	-3.304037	-4.087881	-1.487564
84	1	0	-1.037404	-3.231322	-1.151030
85	1	0	-3.507098	-3.243522	1.823518
86	1	0	-5.755371	-4.227848	1.344183
87	1	0	-7.141091	-0.343563	0.132450
88	1	0	-4.935636	0.608448	0.606056
89	6	0	9.408909	-2.446099	-1.549727
90	1	0	10.412500	-2.209793	-1.901914
91	1	0	9.403974	-2.475049	-0.453941
92	1	0	9.106901	-3.425518	-1.938469
93	6	0	-8.714664	-2.246572	-0.333690
94	1	0	-9.510663	-2.949054	-0.577936
95	1	0	-9.117104	-1.443541	0.292896
96	1	0	-8.297670	-1.820549	-1.253237
97	6	0	-5.731984	-3.905139	-2.144724
98	1	0	-6.795602	-3.986727	-2.367428
99	1	0	-5.150047	-4.417314	-2.919092
100	1	0	-5.530418	-4.359957	-1.169608
101	6	0	-1.526414	8.149989	-1.848683

102	1	0	-1.323772	9.219270	-1.899035
103	1	0	-1.062200	7.649443	-2.706015
104	1	0	-2.609190	7.982003	-1.873893

$5f_{homo}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.984188	-1.961017	1.022883
2	6	0	3.967701	-0.564758	0.952792
3	6	0	5.129612	0.100483	0.535926
4	6	0	6.234272	-0.614481	0.101363
5	6	0	6.210490	-2.010877	0.084035
6	6	0	5.095675	-2.678154	0.590880
7	7	0	2.778586	0.179027	1.156259
8	6	0	2.668446	1.545425	0.630216
9	6	0	1.165788	1.685124	0.320995
10	6	0	0.534359	0.729793	1.315661
11	6	0	1.585605	-0.319376	1.625381
12	7	0	-0.697465	0.814703	1.627212
13	6	0	-1.559316	-0.217916	2.034978
14	6	0	-2.725856	0.153854	2.711104
15	6	0	-3.754292	-0.755375	2.942558
16	6	0	-3.645298	-2.055886	2.443145
17	6	0	-2.483474	-2.439062	1.761459
18	6	0	-1.455056	-1.537846	1.561562
19	8	0	-4.606549	-3.008423	2.558191
20	6	0	-5.826676	-2.629678	3.166403
21	6	0	0.666163	3.128925	0.291666
22	6	0	3.193642	2.584198	1.603568
23	6	0	3.846913	3.714438	1.107392
24	6	0	4.295879	4.708972	1.972092
25	6	0	4.097767	4.578084	3.344809
26	6	0	3.454815	3.448221	3.846439
27	6	0	3.006418	2.453816	2.980675
28	8	0	1.421915	-1.372225	2.217989
29	8	0	7.305042	-2.626132	-0.439440
30	6	0	7.205562	-4.019905	-0.666963
31	6	0	-0.828204	3.257303	-0.070235
32	6	0	-1.314212	2.053120	-0.794674
33	6	0	-0.537905	1.060189	-1.248134
34	6	0	-1.414874	-0.091973	-1.638918
35	7	0	-2.720535	0.296264	-1.362793
36	6	0	-2.757001	1.650907	-0.820725
37	7	0	0.838177	1.036702	-1.016378
38	6	0	1.732699	0.086895	-1.612915
39	6	0	1.669603	-1.289228	-1.351234
40	6	0	2.656317	-2.140983	-1.811265
41	6	0	3.758805	-1.636225	-2.513077
42	6	0	3.807472	-0.279771	-2.833626
43	6	0	2.787119	0.563612	-2.388609
44	8	0	-1.072792	-1.172041	-2.085749
45	6	0	-3.788883	-0.599479	-1.093846
46	6	0	-3.692976	-1.976291	-1.321702
47	6	0	-4.700010	-2.840207	-0.896356
48	6	0	-5.831315	-2.345750	-0.250863
49	6	0	-5.968757	-0.966110	-0.092868
50	6	0	-4.964221	-0.105544	-0.506591
51	6	0	-3.620947	2.617564	-1.610122
52	6	0	-4.313268	3.629148	-0.944543
53	6	0	-5.058158	4.563161	-1.662488
54	6	0	-5.117382	4.485977	-3.051357
55	6	0	-4.427316	3.474409	-3.719336
56	6	0	-3.678625	2.546309	-3.002560
57	8	0	-6.839102	-3.115425	0.247533
58	6	0	-6.606421	-4.509755	0.303965
59	8	0	4.724778	-2.537867	-2.827923
60	6	0	5.923737	-2.032519	-3.385702
61	1	0	3.238650	1.614710	-0.298157
62	1	0	-1.426280	3.361912	0.842066
63	1	0	-0.993542	4.166712	-0.660704
64	1	0	0.851154	3.594965	1.262657
65	1	0	1.280817	3.659151	-0.444755

66	1	0	-3.106135	1.608469	0.223393
67	1	0	4.005398	3.814294	0.035447
68	1	0	4.804863	5.581177	1.574172
69	1	0	4.449662	5.349856	4.021965
70	1	0	3.305213	3.336754	4.915690
71	1	0	2.518602	1.569903	3.382638
72	1	0	-4.274838	3.680747	0.141749
73	1	0	-5.596359	5.344765	-1.135308
74	1	0	-5.702086	5.208121	-3.612480
75	1	0	-4.473389	3.408523	-4.801965
76	1	0	-3.140712	1.755476	-3.518506
77	1	0	-5.103177	0.958093	-0.353443
78	1	0	-6.868824	-0.578659	0.374430
79	1	0	-4.570949	-3.904033	-1.058934
80	1	0	-2.812798	-2.382732	-1.796725
81	1	0	3.110799	-2.493730	1.371625
82	1	0	5.058545	-3.760668	0.621151
83	1	0	7.123802	-0.101490	-0.249973
84	1	0	5.172931	1.184016	0.527205
85	1	0	-0.576081	-1.841265	1.005650
86	1	0	-2.428018	-3.446604	1.362585
87	1	0	-4.644049	-0.429665	3.468001
88	1	0	-2.826324	1.183600	3.042341
89	1	0	2.826234	1.624694	-2.620639
90	1	0	4.632568	0.135798	-3.399486
91	1	0	2.630329	-3.201380	-1.582833
92	1	0	0.848059	-1.686246	-0.766725
93	1	0	8.114799	-4.307204	-1.194931
94	1	0	7.144153	-4.575480	0.275669
95	1	0	6.328075	-4.248225	-1.283691
96	1	0	6.592596	-2.886779	-3.491942
97	1	0	5.745822	-1.585254	-4.370212
98	1	0	6.380160	-1.291840	-2.718423
99	1	0	-6.471378	-3.507481	3.125099
100	1	0	-5.670951	-2.336054	4.210883
101	1	0	-6.298069	-1.807893	2.615995
102	1	0	-7.461463	-4.939702	0.826370
103	1	0	-6.542097	-4.946185	-0.699533
104	1	0	-5.684997	-4.723739	0.858226

5f$_{hetero}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.374160	-3.191086	-0.545514
2	6	0	3.154706	-3.093607	-1.214484
3	6	0	3.023408	-3.687369	-2.477071
4	6	0	4.107620	-4.297279	-3.083584
5	6	0	5.333984	-4.376869	-2.413349
6	6	0	5.459360	-3.834381	-1.131111
7	7	0	1.992688	-2.537921	-0.640634
8	6	0	1.960694	-1.436092	-0.017921
9	6	0	0.679866	-0.927875	0.635123
10	6	0	1.239401	0.184612	1.592387
11	7	0	2.480487	0.607031	0.926560
12	6	0	3.013518	-0.350295	0.104121
13	6	0	-0.054146	-2.085419	1.324153
14	8	0	4.072604	-0.300452	-0.493362
15	6	0	2.940439	1.944741	1.019474
16	6	0	2.446501	2.777342	2.033465
17	6	0	2.778173	4.121715	2.066187
18	6	0	3.619079	4.667971	1.092723
19	6	0	4.139902	3.838303	0.099006
20	6	0	3.804789	2.487289	0.064360
21	6	0	1.490001	-0.240272	3.027197
22	6	0	0.648482	0.217645	4.042830
23	6	0	0.846798	-0.177770	5.363845
24	6	0	1.895599	-1.035700	5.682025
25	6	0	2.747512	-1.489250	4.675893
26	6	0	2.549105	-1.089527	3.357853
27	8	0	3.869633	6.001368	1.194808
28	8	0	6.333663	-5.011066	-3.078563
29	7	0	-0.197685	-0.317317	-0.408745

30	6	0	0.333774	0.836488	-1.085513
31	6	0	1.256134	0.672175	-2.123337
32	6	0	1.874499	1.774999	-2.690733
33	6	0	1.559973	3.067073	-2.252046
34	6	0	0.591716	3.244286	-1.264003
35	6	0	-0.002258	2.126607	-0.682832
36	8	0	2.252166	4.079803	-2.835937
37	6	0	-1.545716	-0.276813	-0.064489
38	6	0	-2.123364	-0.846446	1.002492
39	6	0	-3.615906	-0.653833	0.951031
40	7	0	-3.801614	0.088267	-0.293475
41	6	0	-2.603518	0.310365	-0.947655
42	6	0	-1.374858	-1.679020	1.984101
43	6	0	-4.366663	-1.973270	0.972646
44	6	0	-5.017619	-2.389101	2.132262
45	6	0	-5.657743	-3.627660	2.175367
46	6	0	-5.651122	-4.451851	1.054530
47	6	0	-4.999467	-4.038104	-0.108393
48	6	0	-4.356189	-2.806335	-0.147650
49	6	0	-5.081399	0.481671	-0.749353
50	6	0	-5.329771	0.757049	-2.103619
51	6	0	-6.598865	1.128025	-2.516582
52	6	0	-7.654997	1.221229	-1.604867
53	6	0	-7.418932	0.934877	-0.261675
54	6	0	-6.139429	0.571635	0.155874
55	8	0	-2.453682	0.857957	-2.024234
56	8	0	-8.860204	1.588853	-2.117960
57	1	0	-3.940284	-0.044844	1.807360
58	1	0	0.623241	-2.543066	2.049038
59	1	0	-0.249777	-2.829380	0.546513
60	1	0	-1.206944	-1.146103	2.927822
61	1	0	-1.950470	-2.578497	2.234246
62	1	0	0.541031	1.027634	1.592067
63	1	0	-5.026903	-1.740634	3.005283
64	1	0	-6.164742	-3.942095	3.082337
65	1	0	-6.152993	-5.413849	1.083078
66	1	0	-4.993632	-4.677968	-0.985101
67	1	0	-3.848468	-2.480873	-1.052629
68	1	0	-0.166457	0.896323	3.795356
69	1	0	0.186156	0.190798	6.142443
70	1	0	2.055171	-1.344123	6.710315
71	1	0	3.572994	-2.151163	4.918400
72	1	0	3.230425	-1.437248	2.584999
73	1	0	1.802490	2.378376	2.809347
74	1	0	2.393045	4.769587	2.846626
75	1	0	4.796301	4.228533	-0.670417
76	1	0	4.199296	1.864850	-0.725183
77	1	0	-4.526967	0.686185	-2.823446
78	1	0	-6.796349	1.345221	-3.560839
79	1	0	-8.213099	0.988412	0.473810
80	1	0	-5.984181	0.352198	1.206105
81	1	0	1.499760	-0.328277	-2.469011
82	1	0	2.613685	1.658710	-3.476478
83	1	0	0.314537	4.232342	-0.916855
84	1	0	-0.742236	2.268356	0.102037
85	1	0	2.060970	-3.645805	-2.977505
86	1	0	4.025902	-4.739032	-4.071146
87	1	0	6.392147	-3.901905	-0.583470
88	1	0	4.474916	-2.769828	0.449545
89	6	0	7.591442	-5.099838	-2.437473
90	1	0	8.248784	-5.620399	-3.132427
91	1	0	7.998077	-4.105020	-2.223906
92	1	0	7.521253	-5.670606	-1.504040
93	6	0	-9.943952	1.687302	-1.215715
94	1	0	-10.806766	1.988930	-1.808712
95	1	0	-10.150203	0.723902	-0.735529
96	1	0	-9.750600	2.441512	-0.443475
97	6	0	4.799330	6.558121	0.285253
98	1	0	4.896339	7.608883	0.556642
99	1	0	5.774766	6.066035	0.366663
100	1	0	4.443040	6.481290	-0.748849
101	6	0	1.978441	5.391831	-2.385805
102	1	0	2.648216	6.049258	-2.940424
103	1	0	0.939265	5.673561	-2.590855

104	1	0	2.173740	5.487961	-1.310219

5f$_{homo}$–*exo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.343130	-1.212281	-1.478050
2	6	0	4.266920	-1.884605	-0.905094
3	6	0	4.505130	-3.020631	-0.121582
4	6	0	5.800990	-3.435826	0.130846
5	6	0	6.881955	-2.752945	-0.439573
6	6	0	6.648448	-1.644690	-1.257152
7	7	0	2.917695	-1.552132	-1.156133
8	6	0	2.432485	-0.400443	-0.968018
9	6	0	0.965871	-0.100977	-1.226331
10	6	0	0.988582	1.463555	-1.387936
11	7	0	2.167095	1.857886	-0.596545
12	6	0	3.068724	0.847611	-0.390401
13	6	0	0.456310	-0.849162	-2.469705
14	8	0	4.138642	0.931448	0.181092
15	6	0	2.448492	3.213052	-0.279781
16	6	0	2.109326	4.230813	-1.178295
17	6	0	2.376202	5.552863	-0.867263
18	6	0	2.994852	5.883397	0.344019
19	6	0	3.334976	4.871121	1.242597
20	6	0	3.053817	3.542582	0.929966
21	6	0	-0.262553	2.196512	-0.960456
22	6	0	-1.132335	2.699444	-1.928024
23	6	0	-2.356880	3.255227	-1.561574
24	6	0	-2.710397	3.327455	-0.216156
25	6	0	-1.818314	2.880137	0.758504
26	6	0	-0.594880	2.329965	0.390425
27	8	0	3.218485	7.206183	0.554173
28	8	0	8.114947	-3.248425	-0.151803
29	7	0	0.179126	-0.468808	-0.019041
30	6	0	0.705525	-1.416517	0.919305
31	6	0	1.642094	-1.003293	1.872774
32	6	0	2.200657	-1.916424	2.749166
33	6	0	1.810003	-3.261928	2.709178
34	6	0	0.857202	-3.678396	1.778451
35	6	0	0.321134	-2.751408	0.882938
36	8	0	2.409080	-4.078561	3.614678
37	6	0	-1.184924	-0.556640	-0.279165
38	6	0	-1.774487	-0.550703	-1.478311
39	6	0	-3.264688	-0.415560	-1.311872
40	7	0	-3.428241	-0.396572	0.142533
41	6	0	-2.208879	-0.426116	0.795732
42	6	0	-1.025466	-0.581824	-2.764592
43	6	0	-4.023862	-1.541328	-1.986713
44	6	0	-4.673660	-1.322629	-3.199600
45	6	0	-5.319079	-2.372488	-3.852002
46	6	0	-5.319772	-3.645135	-3.288524
47	6	0	-4.670708	-3.866955	-2.073278
48	6	0	-4.021479	-2.820576	-1.427522
49	6	0	-4.682968	-0.180201	0.753121
50	6	0	-4.894176	-0.478248	2.109513
51	6	0	-6.135089	-0.263213	2.684141
52	6	0	-7.201294	0.237299	1.929683
53	6	0	-7.003665	0.520799	0.580090
54	6	0	-5.750620	0.314108	0.003308
55	8	0	-2.009144	-0.338372	1.993355
56	8	0	-8.377910	0.406369	2.592659
57	1	0	-3.583372	0.549919	-1.733742
58	1	0	0.613120	-1.914576	-2.271990
59	1	0	1.078988	-0.589348	-3.331034
60	1	0	-1.422375	-1.362745	-3.424615
61	1	0	-1.160047	0.368048	-3.299109
62	1	0	1.173684	1.676117	-2.451562
63	1	0	-4.678508	-0.325093	-3.633942
64	1	0	-5.825110	-2.192659	-4.795391
65	1	0	-5.826566	-4.462772	-3.791340
66	1	0	-4.671356	-4.857748	-1.629670
67	1	0	-3.515251	-2.986200	-0.479267

68	1	0	-0.856038	2.644726	-2.979083
69	1	0	-3.030095	3.631488	-2.325879
70	1	0	-3.669468	3.744573	0.074826
71	1	0	-2.083168	2.942900	1.809157
72	1	0	0.086199	1.957968	1.149825
73	1	0	1.630802	3.989522	-2.122212
74	1	0	2.114975	6.352162	-1.552425
75	1	0	3.808804	5.098013	2.189887
76	1	0	3.314409	2.758472	1.630566
77	1	0	-4.080846	-0.866463	2.706429
78	1	0	-6.303719	-0.487712	3.732380
79	1	0	-7.806979	0.902305	-0.038747
80	1	0	-5.626054	0.539962	-1.049806
81	1	0	1.929249	0.043812	1.921496
82	1	0	2.935845	-1.611304	3.486133
83	1	0	0.533025	-4.711066	1.729963
84	1	0	-0.404774	-3.076783	0.141906
85	1	0	3.656066	-3.550684	0.301118
86	1	0	6.003551	-4.298424	0.756949
87	1	0	7.467522	-1.107443	-1.719890
88	1	0	5.161374	-0.346203	-2.106644
89	6	0	9.231170	-2.573274	-0.697417
90	1	0	10.111728	-3.108592	-0.343672
91	1	0	9.209432	-2.591200	-1.793187
92	1	0	9.272622	-1.533574	-0.353321
93	6	0	3.831275	7.576807	1.774550
94	1	0	3.920097	8.662311	1.750996
95	1	0	3.217665	7.278703	2.632186
96	1	0	4.827713	7.130490	1.868950
97	6	0	-9.470097	0.911906	1.851752
98	1	0	-10.305825	0.976782	2.547840
99	1	0	-9.250904	1.908507	1.450940
100	1	0	-9.734429	0.241092	1.025951
101	6	0	2.061010	-5.448729	3.584275
102	1	0	2.649409	-5.928469	4.365588
103	1	0	0.994202	-5.592073	3.790394
104	1	0	2.305834	-5.897531	2.614434

5f$_{hetero}$–*exo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.686605	-1.990079	0.533508
2	6	0	-4.661352	-1.168605	1.002202
3	6	0	-4.937825	-0.282490	2.055989
4	6	0	-6.200983	-0.246659	2.621444
5	6	0	-7.225081	-1.074220	2.149798
6	6	0	-6.962071	-1.946352	1.095437
7	7	0	-3.387031	-1.216158	0.393022
8	6	0	-3.202293	-1.703100	-0.980178
9	6	0	-1.726293	-1.520944	-1.194937
10	6	0	-1.188196	-0.915695	-0.135820
11	6	0	-2.208678	-0.722410	0.928170
12	6	0	-0.901823	-1.745675	-2.417804
13	6	0	-0.057389	-0.477724	-2.611870
14	6	0	0.714778	-0.007956	-1.358610
15	7	0	0.113365	-0.433069	-0.061120
16	6	0	0.840821	1.547376	-1.397787
17	7	0	2.055306	1.777983	-0.600234
18	6	0	2.938026	0.720892	-0.660917
19	6	0	2.173750	-0.420317	-1.320977
20	7	0	2.572838	-1.515244	-1.815869
21	6	0	3.873892	-2.029818	-1.631266
22	6	0	4.463044	-2.114440	-0.369309
23	6	0	5.689971	-2.748662	-0.199275
24	6	0	6.347380	-3.294340	-1.305069
25	6	0	5.753314	-3.223981	-2.571173
26	6	0	4.516264	-2.622288	-2.725499
27	8	0	7.550594	-3.923090	-1.248574
28	6	0	-0.398086	2.294847	-0.966450
29	6	0	-1.126973	2.984654	-1.940368
30	6	0	-2.301631	3.658211	-1.613440
31	6	0	-2.772201	3.634508	-0.302946

32	6	0	-2.052542	2.948606	0.675051
33	6	0	-0.866392	2.294648	0.351393
34	6	0	2.441452	3.059577	-0.131080
35	6	0	2.060306	4.217425	-0.818641
36	6	0	2.423282	5.464774	-0.339449
37	6	0	3.183424	5.580964	0.829400
38	6	0	3.572754	4.428725	1.514574
39	6	0	3.196095	3.176470	1.034684
40	8	0	4.094532	0.732543	-0.289582
41	8	0	3.491344	6.846514	1.214548
42	6	0	0.922297	-1.018209	0.975595
43	6	0	1.602800	-0.217612	1.898997
44	6	0	2.404691	-0.791554	2.873330
45	6	0	2.525437	-2.183925	2.958429
46	6	0	1.827553	-2.994721	2.059557
47	6	0	1.039780	-2.403084	1.074730
48	8	0	3.336885	-2.650527	3.940996
49	6	0	-3.996088	-0.898098	-1.994938
50	6	0	-4.761783	-1.532253	-2.969664
51	6	0	-5.445216	-0.779871	-3.925486
52	6	0	-5.364977	0.608956	-3.903823
53	6	0	-4.595236	1.245733	-2.928474
54	6	0	-3.908308	0.496433	-1.981047
55	8	0	-2.042361	-0.230229	2.030882
56	8	0	-8.428649	-0.953816	2.773401
57	1	0	-3.477276	-2.763585	-1.050548
58	1	0	0.662170	-0.608951	-3.425147
59	1	0	-0.747109	0.325393	-2.899084
60	1	0	-0.247112	-2.615844	-2.283239
61	1	0	-1.520518	-1.923918	-3.302657
62	1	0	1.048931	1.826205	-2.442007
63	1	0	-4.828495	-2.617997	-2.981095
64	1	0	-6.042857	-1.280993	-4.680512
65	1	0	-5.900220	1.196420	-4.643269
66	1	0	-4.527518	2.329064	-2.905895
67	1	0	-3.302623	0.992670	-1.223206
68	1	0	-0.763601	3.003072	-2.965924
69	1	0	-2.844130	4.200681	-2.381858
70	1	0	-3.691925	4.149396	-0.043065
71	1	0	-2.412119	2.919379	1.698819
72	1	0	-0.326748	1.758891	1.122865
73	1	0	1.475132	4.144888	-1.729214
74	1	0	2.129988	6.369756	-0.860704
75	1	0	4.161941	4.487552	2.421659
76	1	0	3.504539	2.283073	1.565651
77	1	0	-4.157817	0.366310	2.429140
78	1	0	-6.420410	0.433453	3.438109
79	1	0	-7.730776	-2.598704	0.698874
80	1	0	-5.508379	-2.678994	-0.284730
81	1	0	1.509376	0.862634	1.844108
82	1	0	2.942877	-0.179066	3.589243
83	1	0	1.901205	-4.074621	2.102963
84	1	0	0.511900	-3.029785	0.360636
85	1	0	4.036129	-2.590692	-3.698626
86	1	0	6.273828	-3.666569	-3.413889
87	1	0	6.120286	-2.804274	0.793630
88	1	0	3.949654	-1.688128	0.487027
89	6	0	-9.478865	-1.782162	2.316691
90	1	0	-10.344429	-1.544014	2.934146
91	1	0	-9.714603	-1.581273	1.265083
92	1	0	-9.227712	-2.842784	2.434005
93	6	0	3.535857	-4.049839	4.010739
94	1	0	4.231712	-4.215780	4.832292
95	1	0	2.596572	-4.575056	4.216694
96	1	0	3.969315	-4.432334	3.079207
97	6	0	8.184946	-4.001996	0.013167
98	1	0	9.127365	-4.522527	-0.153667
99	1	0	8.384812	-3.003928	0.419016
100	1	0	7.576928	-4.568172	0.728142
101	6	0	4.255722	6.999596	2.395153
102	1	0	4.393256	8.071902	2.529633
103	1	0	3.730000	6.586834	3.263636
104	1	0	5.233872	6.514779	2.299342

RCg$_{homo}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.860733	-0.172181	1.139446
2	6	0	-1.975630	1.070379	1.776618
3	6	0	-3.133090	1.346220	2.518633
4	6	0	-4.130796	0.391663	2.669118
5	6	0	-3.992018	-0.832742	2.024706
6	6	0	-2.869812	-1.119564	1.255748
7	7	0	-1.080659	2.145746	1.627390
8	6	0	0.192801	2.100738	1.615239
9	6	0	1.030301	3.296468	1.437051
10	6	0	2.474886	2.868833	1.324451
11	7	0	2.412642	1.421864	1.611009
12	6	0	1.144843	0.931875	1.809142
13	6	0	0.566880	4.545369	1.420103
14	8	0	0.842181	-0.215152	2.083666
15	6	0	3.564720	0.605544	1.521226
16	6	0	4.638170	1.016052	0.721099
17	6	0	5.756167	0.206728	0.567905
18	6	0	5.804238	-1.019205	1.219273
19	6	0	4.757730	-1.434256	2.032379
20	6	0	3.641221	-0.620963	2.192832
21	6	0	3.397192	3.600447	2.294450
22	35	0	7.310465	-2.140007	0.988827
23	35	0	-5.395490	-2.097429	2.118967
24	6	0	-0.567146	4.547981	-1.415457
25	6	0	-1.030387	3.299030	-1.433660
26	6	0	-0.192778	2.103594	-1.613353
27	6	0	-1.144759	0.934829	-1.808252
28	7	0	-2.412546	1.424440	-1.609177
29	6	0	-2.474895	2.871093	-1.321073
30	7	0	1.080681	2.148767	-1.625835
31	6	0	1.975625	1.073510	-1.776036
32	6	0	1.860489	-0.169595	-1.139982
33	6	0	2.869390	-1.117059	-1.257046
34	6	0	3.991707	-0.829724	-2.025656
35	6	0	4.130774	0.395270	-2.668890
36	6	0	3.133219	1.349876	-2.517638
37	6	0	-3.397600	3.603600	-2.290016
38	6	0	-3.564523	0.607875	-1.520253
39	6	0	-3.641105	-0.617620	-2.193696
40	6	0	-4.757500	-1.431243	-2.034169
41	6	0	-5.803814	-1.017518	-1.220137
42	6	0	-5.755671	0.207439	-0.566936
43	6	0	-4.637780	1.017091	-0.719216
44	8	0	-0.842103	-0.211840	-2.084284
45	35	0	-7.309907	-2.138799	-0.991080
46	35	0	5.394876	-2.094664	-2.121112
47	1	0	-2.806780	3.010690	-0.284048
48	1	0	1.219303	5.404891	1.299219
49	1	0	-0.498012	4.723283	1.532962
50	1	0	0.497688	4.726194	-1.528402
51	1	0	-1.219674	5.407264	-1.293428
52	1	0	2.807068	3.009563	0.287671
53	1	0	4.599582	1.954290	0.179691
54	1	0	6.573600	0.518856	-0.073023
55	1	0	4.811258	-2.388693	2.543983
56	1	0	2.826170	-0.946474	2.822392
57	1	0	-2.826208	-0.942099	-2.823988
58	1	0	-4.811106	-2.384898	-2.547220
59	1	0	-6.572949	0.518525	0.074698
60	1	0	-4.599083	1.954504	-0.176382
61	1	0	0.996645	-0.394337	-0.527617
62	1	0	2.791994	-2.065014	-0.736061
63	1	0	5.019268	0.609287	-3.252514
64	1	0	3.232826	2.327118	-2.979479
65	1	0	-3.232477	2.323057	2.981378
66	1	0	-5.019197	0.605301	3.253022
67	1	0	-2.792626	-2.067055	0.733894
68	1	0	-0.997127	-0.396542	0.526592
69	1	0	-4.422872	3.231806	-2.226580

70	1	0	-3.406646	4.670423	-2.052241
71	1	0	-3.037856	3.475300	-3.314412
72	1	0	4.422523	3.228822	2.231006
73	1	0	3.406218	4.667511	2.057755
74	1	0	3.037095	3.471078	3.318587

RCg_{hetero}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.046625	2.042435	2.867204
2	6	0	1.398019	0.850292	2.222546
3	6	0	2.482092	0.845163	1.339129
4	6	0	3.167081	2.018349	1.045888
5	6	0	2.789766	3.193718	1.683187
6	6	0	1.743354	3.212975	2.601456
7	7	0	0.806954	-0.391035	2.525355
8	6	0	-0.447999	-0.608849	2.553838
9	6	0	-1.044165	-1.885864	2.963329
10	6	0	-2.500368	-1.888240	2.560239
11	7	0	-2.709270	-0.519504	2.045609
12	6	0	-1.585660	0.272831	2.065699
13	6	0	-0.393878	-2.843571	3.622588
14	8	0	-1.494683	1.426940	1.692798
15	6	0	-3.902870	-0.165677	1.373679
16	6	0	-4.750886	-1.168962	0.891192
17	6	0	-5.888311	-0.844650	0.159856
18	6	0	-6.184155	0.487428	-0.085243
19	6	0	-5.375186	1.499850	0.416677
20	6	0	-4.243081	1.178300	1.152491
21	6	0	-3.447594	-2.212236	3.711298
22	35	0	-7.682470	0.933872	-1.148932
23	35	0	3.731882	4.796654	1.314396
24	6	0	0.796617	-4.646506	1.409158
25	6	0	1.338668	-3.648036	0.713858
26	6	0	0.585908	-2.690358	-0.108272
27	6	0	1.612503	-1.860268	-0.861704
28	7	0	2.848797	-2.242331	-0.389612
29	6	0	2.809203	-3.309613	0.631417
30	7	0	-0.685382	-2.675713	-0.174692
31	6	0	-1.459755	-1.749162	-0.898294
32	6	0	-1.247128	-0.365716	-0.866502
33	6	0	-2.148730	0.496712	-1.475913
34	6	0	-3.242946	-0.029010	-2.157381
35	6	0	-3.462895	-1.400166	-2.218830
36	6	0	-2.586984	-2.253189	-1.558631
37	6	0	3.371321	-2.843603	1.973740
38	6	0	4.075459	-1.715308	-0.857975
39	6	0	4.144513	-0.445765	-1.451580
40	6	0	5.366430	0.061413	-1.878221
41	6	0	6.523491	-0.690144	-1.714405
42	6	0	6.474464	-1.947097	-1.126556
43	6	0	5.253481	-2.455914	-0.700440
44	8	0	1.391032	-1.050853	-1.740573
45	35	0	8.185170	0.008032	-2.294088
46	35	0	-4.477398	1.142671	-2.986262
47	1	0	3.365919	-4.176417	0.259208
48	1	0	-0.878173	-3.765334	3.931246
49	1	0	0.655867	-2.713580	3.868318
50	1	0	-0.278762	-4.794440	1.387648
51	1	0	1.398438	-5.334829	1.995507
52	1	0	-2.629546	-2.596277	1.731662
53	1	0	-4.521907	-2.216445	1.045175
54	1	0	-6.526691	-1.629255	-0.230849
55	1	0	-5.620794	2.538368	0.224751
56	1	0	-3.610976	1.966448	1.532584
57	1	0	3.247097	0.141501	-1.587920
58	1	0	5.413093	1.043171	-2.336413
59	1	0	7.380232	-2.529178	-1.000517
60	1	0	5.235357	-3.438542	-0.244224
61	1	0	-0.389675	0.042302	-0.341456
62	1	0	-2.003615	1.569618	-1.415087
63	1	0	-4.328227	-1.790580	-2.743087

64	1	0	-2.760803	-3.324713	-1.553323
65	1	0	2.786096	-0.091790	0.884809
66	1	0	3.996626	2.010744	0.346647
67	1	0	1.473441	4.137375	3.099615
68	1	0	0.226456	2.047497	3.576359
69	1	0	-4.493217	-2.136951	3.403599
70	1	0	-3.267149	-3.231763	4.062097
71	1	0	-3.274011	-1.520465	4.539841
72	1	0	4.403141	-2.494962	1.877759
73	1	0	2.749120	-2.034961	2.370165
74	1	0	3.354326	-3.677536	2.681372

RCg$_{homo}$-in/in

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.570630	1.430867	-2.981425
2	6	0	-1.081301	0.365121	-2.229090
3	6	0	-2.262486	0.551989	-1.500565
4	6	0	-2.886323	1.793314	-1.459457
5	6	0	-2.346891	2.842063	-2.193886
6	6	0	-1.201907	2.667008	-2.965833
7	7	0	-0.556313	-0.939119	-2.279411
8	6	0	0.680346	-1.235098	-2.191474
9	6	0	1.201027	-2.599482	-2.367549
10	6	0	2.678222	-2.610936	-2.038104
11	7	0	2.938990	-1.205307	-1.675396
12	6	0	1.866094	-0.360547	-1.809512
13	6	0	0.476500	-3.636594	-2.785098
14	8	0	1.862928	0.840551	-1.619453
15	6	0	4.214476	-0.776831	-1.237705
16	6	0	5.369364	-1.390295	-1.730731
17	6	0	6.621545	-1.004825	-1.263879
18	6	0	6.712637	-0.004820	-0.303045
19	6	0	5.573707	0.616688	0.195673
20	6	0	4.325663	0.231457	-0.276375
21	6	0	3.033209	-3.576112	-0.910399
22	35	0	8.416984	0.509622	0.347104
23	35	0	-3.202011	4.532698	-2.165398
24	6	0	-0.692880	-4.653363	-0.134806
25	6	0	-1.356401	-3.553295	0.216965
26	6	0	-0.754386	-2.364456	0.836743
27	6	0	-1.907332	-1.482849	1.291163
28	7	0	-3.054748	-2.051107	0.785890
29	6	0	-2.841000	-3.317823	0.057319
30	7	0	0.500737	-2.206948	0.979525
31	6	0	1.124490	-1.061932	1.508544
32	6	0	0.777035	0.248916	1.159861
33	6	0	1.514264	1.321369	1.645591
34	6	0	2.601677	1.078511	2.478837
35	6	0	2.969718	-0.214083	2.835062
36	6	0	2.240150	-1.281240	2.327115
37	6	0	-3.256240	-3.216322	-1.409916
38	6	0	-4.348949	-1.508424	0.962779
39	6	0	-4.534020	-0.135831	1.182677
40	6	0	-5.815584	0.383752	1.319763
41	6	0	-6.916037	-0.460722	1.236322
42	6	0	-6.751286	-1.822244	1.018504
43	6	0	-5.469760	-2.342847	0.882732
44	8	0	-1.838867	-0.493900	1.993760
45	35	0	-8.660394	0.253411	1.417925
46	35	0	3.689285	2.529494	3.028507
47	1	0	-3.398842	-4.114812	0.560502
48	1	0	0.908072	-4.624145	-2.922072
49	1	0	-0.578513	-3.506395	-3.006290
50	1	0	0.378166	-4.716478	0.030761
51	1	0	-1.193748	-5.508890	-0.579301
52	1	0	3.253865	-2.857901	-2.938920
53	1	0	5.301556	-2.171906	-2.480238
54	1	0	7.517891	-1.480493	-1.645139
55	1	0	5.645804	1.383341	0.960515
56	1	0	3.434488	0.708618	0.105957
57	1	0	-3.679246	0.522286	1.258876

58	1	0	-5.953628	1.445855	1.489493
59	1	0	-7.614012	-2.475589	0.955885
60	1	0	-5.357954	-3.407710	0.714715
61	1	0	-0.051531	0.432260	0.483559
62	1	0	1.265341	2.334448	1.350310
63	1	0	3.834746	-0.383406	3.466275
64	1	0	2.524163	-2.302149	2.562248
65	1	0	-2.694936	-0.291101	-0.971111
66	1	0	-3.795007	1.935081	-0.884271
67	1	0	-0.806052	3.491859	-3.547647
68	1	0	0.321260	1.287110	-3.579818
69	1	0	-4.305128	-2.924573	-1.510478
70	1	0	-2.623844	-2.483664	-1.921899
71	1	0	-3.122909	-4.189601	-1.891294
72	1	0	4.097926	-3.530708	-0.667832
73	1	0	2.443607	-3.332907	-0.021936
74	1	0	2.799813	-4.597650	-1.225170

TSg_{homo}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.747951	-0.371686	1.190825
2	6	0	-1.887916	0.940902	1.672690
3	6	0	-3.101002	1.305078	2.283075
4	6	0	-4.132878	0.390679	2.440200
5	6	0	-3.976855	-0.891380	1.924815
6	6	0	-2.794733	-1.277322	1.299211
7	7	0	-0.984654	1.989230	1.485625
8	6	0	0.308634	1.953832	1.458336
9	6	0	1.053567	3.124367	1.134430
10	6	0	2.522209	2.812601	1.108831
11	7	0	2.551275	1.378760	1.457544
12	6	0	1.303715	0.838461	1.684429
13	6	0	0.412168	4.331889	0.892784
14	8	0	1.052234	-0.308306	2.009747
15	6	0	3.745211	0.624904	1.389374
16	6	0	4.845781	1.131800	0.686124
17	6	0	6.009027	0.384413	0.549143
18	6	0	6.080795	-0.877196	1.121783
19	6	0	5.011926	-1.388786	1.845160
20	6	0	3.850753	-0.638774	1.990149
21	6	0	3.320663	3.652746	2.106377
22	35	0	7.639671	-1.922525	0.885141
23	35	0	-5.421041	-2.108439	2.019656
24	6	0	-0.412176	4.331692	-0.893733
25	6	0	-1.053557	3.124099	-1.135084
26	6	0	-0.308593	1.953494	-1.458648
27	6	0	-1.303646	0.838056	-1.684530
28	7	0	-2.551221	1.378372	-1.457764
29	6	0	-2.522183	2.812282	-1.109311
30	7	0	0.984698	1.988916	-1.485926
31	6	0	1.887981	0.940557	-1.672713
32	6	0	1.748001	-0.371921	-1.190553
33	6	0	2.794728	-1.277628	-1.298850
34	6	0	3.976828	-0.891855	-1.924603
35	6	0	4.132890	0.390107	-2.440212
36	6	0	3.101056	1.304578	-2.283207
37	6	0	-3.320805	3.652210	-2.106899
38	6	0	-3.745160	0.624542	-1.389472
39	6	0	-3.850694	-0.639251	-1.990002
40	6	0	-5.011860	-1.389248	-1.844862
41	6	0	-6.080749	-0.877500	-1.121632
42	6	0	-6.008977	0.384208	-0.549206
43	6	0	-4.845722	1.131558	-0.686290
44	8	0	-1.052140	-0.308754	-2.009675
45	35	0	-7.639667	-1.922745	-0.884894
46	35	0	5.420919	-2.109040	-2.019358
47	1	0	-2.910269	2.942631	-0.089848
48	1	0	1.007422	5.235378	0.788572
49	1	0	-0.544850	4.448790	1.394324
50	1	0	0.544841	4.448466	-1.395303
51	1	0	-1.007433	5.235198	-0.789710

52	1	0	2.910388	2.942826	0.089389
53	1	0	4.799292	2.100685	0.203961
54	1	0	6.845377	0.776776	-0.018850
55	1	0	5.080450	-2.372135	2.296869
56	1	0	3.021197	-1.042486	2.550329
57	1	0	-3.021142	-1.043054	-2.550123
58	1	0	-5.080389	-2.372671	-2.296407
59	1	0	-6.845340	0.776677	0.018696
60	1	0	-4.799244	2.100554	-0.204344
61	1	0	0.829096	-0.678133	-0.709613
62	1	0	2.697480	-2.276911	-0.889045
63	1	0	5.062899	0.677332	-2.918633
64	1	0	3.210853	2.324783	-2.638409
65	1	0	-3.210786	2.325358	2.638068
66	1	0	-5.062895	0.678031	2.918530
67	1	0	-2.697502	-2.276682	0.889591
68	1	0	-0.829041	-0.678015	0.709969
69	1	0	-4.370809	3.351100	-2.132453
70	1	0	-3.272119	4.706799	-1.822820
71	1	0	-2.898606	3.537851	-3.108863
72	1	0	4.370640	3.351580	2.132244
73	1	0	3.272109	4.707263	1.822003
74	1	0	2.898230	3.538684	3.108275

TSg_{hetero}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.012519	2.440090	2.445012
2	6	0	1.451727	1.197323	1.965039
3	6	0	2.589598	1.154131	1.150642
4	6	0	3.239242	2.320413	0.763335
5	6	0	2.771224	3.540055	1.234530
6	6	0	1.669869	3.607291	2.084062
7	7	0	0.896855	-0.022945	2.382400
8	6	0	-0.369101	-0.266942	2.411568
9	6	0	-0.913121	-1.482093	2.935281
10	6	0	-2.401235	-1.507133	2.728698
11	7	0	-2.654703	-0.252047	1.996133
12	6	0	-1.525985	0.521441	1.826768
13	6	0	-0.133655	-2.411494	3.618368
14	8	0	-1.450558	1.600032	1.270272
15	6	0	-3.893248	-0.009231	1.358994
16	6	0	-4.846505	-1.033600	1.276044
17	6	0	-6.025519	-0.853482	0.562137
18	6	0	-6.263835	0.359016	-0.067757
19	6	0	-5.359972	1.406401	0.049922
20	6	0	-4.183595	1.230664	0.766009
21	6	0	-3.180573	-1.559350	4.044878
22	35	0	-7.811177	0.579238	-1.133562
23	35	0	3.657830	5.138631	0.731113
24	6	0	0.613467	-3.716707	2.413640
25	6	0	1.306240	-3.072753	1.394970
26	6	0	0.621785	-2.392748	0.356136
27	6	0	1.671035	-1.794324	-0.555598
28	7	0	2.892798	-2.106186	0.012028
29	6	0	2.790546	-2.910076	1.242839
30	7	0	-0.676120	-2.380689	0.323407
31	6	0	-1.478403	-1.680631	-0.583696
32	6	0	-1.230464	-0.380017	-1.054767
33	6	0	-2.175918	0.272995	-1.832550
34	6	0	-3.357889	-0.381954	-2.174751
35	6	0	-3.616990	-1.676271	-1.742409
36	6	0	-2.687056	-2.306487	-0.926105
37	6	0	3.470619	-2.260229	2.447166
38	6	0	4.140100	-1.780200	-0.566092
39	6	0	4.287819	-0.640322	-1.369578
40	6	0	5.529902	-0.317709	-1.903352
41	6	0	6.628254	-1.125350	-1.633872
42	6	0	6.500831	-2.256714	-0.838857
43	6	0	5.257801	-2.582586	-0.309166
44	8	0	1.497550	-1.198080	-1.600493
45	35	0	8.321342	-0.675686	-2.354763

46	35	0	-4.663856	0.520672	-3.204855
47	1	0	3.235065	-3.897599	1.057697
48	1	0	-0.639617	-3.134609	4.253815
49	1	0	0.804909	-2.030063	4.011707
50	1	0	-0.355349	-4.116993	2.124252
51	1	0	1.174431	-4.315495	3.127718
52	1	0	-2.664360	-2.354953	2.081005
53	1	0	-4.667668	-2.002419	1.725388
54	1	0	-6.740589	-1.664543	0.480347
55	1	0	-5.560065	2.355555	-0.434700
56	1	0	-3.477422	2.043097	0.835330
57	1	0	3.433428	-0.012130	-1.583038
58	1	0	5.640082	0.564868	-2.523669
59	1	0	7.361715	-2.883348	-0.635092
60	1	0	5.170206	-3.472686	0.303547
61	1	0	-0.318755	0.134932	-0.775708
62	1	0	-2.003242	1.291253	-2.162963
63	1	0	-4.548084	-2.165016	-2.007183
64	1	0	-2.878918	-3.303315	-0.540440
65	1	0	2.961822	0.191492	0.819736
66	1	0	4.108855	2.275522	0.116116
67	1	0	1.328370	4.566470	2.457081
68	1	0	0.154080	2.486404	3.105717
69	1	0	-4.256383	-1.470499	3.876347
70	1	0	-2.990805	-2.508242	4.553660
71	1	0	-2.861520	-0.741006	4.695925
72	1	0	4.535386	-2.100524	2.258723
73	1	0	2.988124	-1.307103	2.674640
74	1	0	3.376607	-2.920050	3.315430

TSg$_{homo}$-in/in

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.567747	1.659656	-2.792601
2	6	0	-1.150201	0.578272	-2.112775
3	6	0	-2.373295	0.779605	-1.457310
4	6	0	-2.967242	2.035090	-1.411547
5	6	0	-2.354742	3.093784	-2.069759
6	6	0	-1.167019	2.910935	-2.772939
7	7	0	-0.656987	-0.732948	-2.173764
8	6	0	0.594001	-1.046869	-2.075369
9	6	0	1.059560	-2.388857	-2.237609
10	6	0	2.549442	-2.454562	-2.039620
11	7	0	2.866183	-1.083502	-1.613304
12	6	0	1.803327	-0.212747	-1.678972
13	6	0	0.222734	-3.447795	-2.586841
14	8	0	1.837860	0.978232	-1.437416
15	6	0	4.168038	-0.693253	-1.225848
16	6	0	5.287101	-1.285627	-1.816626
17	6	0	6.567241	-0.940924	-1.394960
18	6	0	6.721218	-0.000041	-0.383992
19	6	0	5.618044	0.604287	0.208692
20	6	0	4.342237	0.258927	-0.217326
21	6	0	3.008357	-3.523597	-1.051556
22	35	0	8.464944	0.457351	0.202735
23	35	0	-3.160433	4.809050	-2.031574
24	6	0	-0.544217	-4.230511	-1.040983
25	6	0	-1.316813	-3.293105	-0.357044
26	6	0	-0.748823	-2.299264	0.481271
27	6	0	-1.899754	-1.489943	1.048866
28	7	0	-3.047625	-1.992427	0.466748
29	6	0	-2.807296	-3.128570	-0.436753
30	7	0	0.531666	-2.227202	0.684079
31	6	0	1.163686	-1.186565	1.374952
32	6	0	0.812020	0.169090	1.270806
33	6	0	1.566834	1.142868	1.911660
34	6	0	2.677618	0.763323	2.658854
35	6	0	3.046131	-0.572082	2.786343
36	6	0	2.297754	-1.536179	2.126562
37	6	0	-3.327465	-2.888684	-1.854394
38	6	0	-4.350289	-1.533743	0.764721
39	6	0	-4.573967	-0.207086	1.160154

40	6	0	-5.864875	0.235899	1.422078
41	6	0	-6.936091	-0.638595	1.284359
42	6	0	-6.733616	-1.954227	0.888738
43	6	0	-5.441978	-2.399276	0.632262
44	8	0	-1.850336	-0.613322	1.888619
45	35	0	-8.694009	-0.029783	1.640416
46	35	0	3.791590	2.100339	3.406654
47	1	0	-3.284692	-4.024190	-0.015799
48	1	0	0.695108	-4.352241	-2.965826
49	1	0	-0.696623	-3.166811	-3.093810
50	1	0	0.390364	-4.499937	-0.555406
51	1	0	-1.065406	-5.055321	-1.523007
52	1	0	3.024153	-2.641328	-3.015066
53	1	0	5.167534	-2.017619	-2.609073
54	1	0	7.436408	-1.401125	-1.850891
55	1	0	5.740957	1.323002	1.012494
56	1	0	3.477065	0.721391	0.237238
57	1	0	-3.740625	0.473221	1.274403
58	1	0	-6.033568	1.261954	1.729630
59	1	0	-7.574220	-2.630839	0.784601
60	1	0	-5.296822	-3.430849	0.331834
61	1	0	-0.031307	0.466726	0.657064
62	1	0	1.314821	2.191476	1.800925
63	1	0	3.924165	-0.845810	3.360395
64	1	0	2.576740	-2.583171	2.191945
65	1	0	-2.859533	-0.065208	-0.982856
66	1	0	-3.905258	2.180666	-0.886113
67	1	0	-0.713270	3.742998	-3.299755
68	1	0	0.354489	1.515222	-3.342160
69	1	0	-4.403196	-2.695255	-1.849591
70	1	0	-2.802706	-2.041540	-2.302982
71	1	0	-3.149218	-3.780325	-2.464018
72	1	0	4.094406	-3.511117	-0.935038
73	1	0	2.530450	-3.361845	-0.084288
74	1	0	2.724211	-4.510171	-1.431815

5g$_{homo}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.060260	-0.118734	-1.058537
2	6	0	2.031901	1.270166	-1.206732
3	6	0	3.113719	1.912721	-1.815746
4	6	0	4.242705	1.195607	-2.203046
5	6	0	4.267739	-0.178132	-1.991625
6	6	0	3.174810	-0.848783	-1.455187
7	7	0	0.981550	2.062938	-0.646760
8	6	0	-0.295879	2.181841	-1.181478
9	6	0	-1.098604	3.216114	-0.897114
10	6	0	-2.523345	2.868621	-1.201489
11	7	0	-2.428503	1.501816	-1.725918
12	6	0	-1.113320	1.051062	-1.706527
13	6	0	-0.691608	4.401417	-0.088615
14	8	0	-0.728159	-0.068543	-1.993706
15	6	0	-3.540027	0.631486	-1.727134
16	6	0	-4.707891	0.980573	-1.033660
17	6	0	-5.770235	0.090762	-0.936938
18	6	0	-5.672370	-1.157784	-1.535838
19	6	0	-4.540950	-1.508111	-2.261457
20	6	0	-3.481778	-0.613417	-2.369557
21	6	0	-3.224931	3.816590	-2.168818
22	35	0	-7.095204	-2.393499	-1.352558
23	35	0	5.848283	-1.151751	-2.361024
24	6	0	0.695919	4.200382	0.567654
25	6	0	1.090898	2.730313	0.698562
26	6	0	0.204419	1.829549	1.537629
27	6	0	1.082309	0.667573	1.970915
28	7	0	2.384299	1.064812	1.748743
29	6	0	2.472355	2.475123	1.310861
30	7	0	-1.045272	2.013190	1.657068
31	6	0	-2.010652	1.023402	1.920796
32	6	0	-2.009702	-0.183842	1.208397
33	6	0	-3.106790	-1.032805	1.258715

34	6	0	-4.203229	-0.680540	2.037634
35	6	0	-4.217548	0.501392	2.770981
36	6	0	-3.127709	1.361531	2.693152
37	6	0	2.809153	3.382538	2.489493
38	6	0	3.508751	0.209260	1.705450
39	6	0	3.391203	-1.172528	1.924820
40	6	0	4.472116	-2.012480	1.684290
41	6	0	5.678706	-1.485617	1.241659
42	6	0	5.834230	-0.115410	1.088433
43	6	0	4.756700	0.727782	1.330393
44	8	0	0.699946	-0.385464	2.443665
45	35	0	7.118582	-2.639987	0.828197
46	35	0	-5.732732	-1.796588	2.022967
47	1	0	3.235648	2.564253	0.538978
48	1	0	-1.450997	4.554487	0.685521
49	1	0	-0.678087	5.310781	-0.701425
50	1	0	0.700503	4.673940	1.553013
51	1	0	1.473446	4.685368	-0.033758
52	1	0	-3.049032	2.846939	-0.235557
53	1	0	-4.796783	1.936124	-0.531179
54	1	0	-6.656164	0.359353	-0.372008
55	1	0	-4.481924	-2.477678	-2.743764
56	1	0	-2.599761	-0.890950	-2.927892
57	1	0	2.450266	-1.592939	2.246906
58	1	0	4.364637	-3.082182	1.826770
59	1	0	6.783560	0.295655	0.763289
60	1	0	4.908831	1.791852	1.198906
61	1	0	-1.166169	-0.433252	0.572204
62	1	0	-3.124249	-1.943989	0.670295
63	1	0	-5.084489	0.762683	3.367611
64	1	0	-3.140406	2.312048	3.217050
65	1	0	3.079283	2.990289	-1.950230
66	1	0	5.098005	1.699155	-2.639342
67	1	0	3.214610	-1.921213	-1.300514
68	1	0	1.220333	-0.623965	-0.593889
69	1	0	3.722421	3.028524	2.975262
70	1	0	2.972515	4.410610	2.156794
71	1	0	2.004609	3.372818	3.232043
72	1	0	-4.249868	3.488780	-2.363350
73	1	0	-3.259912	4.824262	-1.744708
74	1	0	-2.680124	3.849125	-3.115961

5g$_{hetero}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.800476	4.685283	0.771083
2	6	0	0.067968	3.624578	0.503207
3	6	0	0.895681	3.668850	-0.620166
4	6	0	0.823380	4.743413	-1.499394
5	6	0	-0.053543	5.786341	-1.225376
6	6	0	-0.861731	5.770637	-0.093467
7	7	0	0.224654	2.554458	1.413258
8	6	0	-0.696993	1.718704	1.646275
9	6	0	-0.567006	0.542003	2.600431
10	6	0	-2.055476	0.194636	2.854693
11	7	0	-2.728726	0.603948	1.602983
12	6	0	-2.038532	1.587201	0.939524
13	6	0	0.216032	0.848295	3.884920
14	8	0	-2.368960	2.188572	-0.063171
15	6	0	-3.813321	-0.128960	1.070519
16	6	0	-4.430758	-1.116883	1.848954
17	6	0	-5.355534	-1.987591	1.283685
18	6	0	-5.684273	-1.856527	-0.058123
19	6	0	-5.149950	-0.826394	-0.821305
20	6	0	-4.221513	0.040452	-0.262099
21	6	0	-2.691344	0.905729	4.046068
22	35	0	-6.840360	-3.111216	-0.873449
23	35	0	-0.142130	7.265397	-2.409523
24	6	0	1.690725	1.199992	3.639896
25	6	0	2.238737	0.311207	2.581046
26	6	0	1.477185	-0.473256	1.805250
27	6	0	2.352417	-1.259784	0.885910

28	7	0	3.643107	-0.823054	1.137853
29	6	0	3.684266	0.180903	2.204967
30	7	0	0.092880	-0.597592	1.889566
31	6	0	-0.619136	-1.263951	0.831819
32	6	0	-0.668688	-0.742739	-0.464785
33	6	0	-1.453207	-1.351926	-1.435475
34	6	0	-2.180396	-2.494036	-1.101780
35	6	0	-2.105990	-3.053642	0.164217
36	6	0	-1.313619	-2.433156	1.128776
37	6	0	4.279061	1.507521	1.732744
38	6	0	4.800669	-1.323378	0.513747
39	6	0	4.750178	-1.882319	-0.771543
40	6	0	5.908537	-2.356215	-1.374572
41	6	0	7.123930	-2.264575	-0.706861
42	6	0	7.195945	-1.706853	0.562297
43	6	0	6.035393	-1.242438	1.170513
44	8	0	2.024842	-2.121045	0.090323
45	35	0	8.702565	-2.904124	-1.540387
46	35	0	-3.334541	-3.273519	-2.384393
47	1	0	4.259159	-0.208458	3.056333
48	1	0	0.150019	-0.041139	4.522314
49	1	0	-0.271870	1.671219	4.411688
50	1	0	2.251309	1.081069	4.574938
51	1	0	1.785704	2.248477	3.336239
52	1	0	-2.146873	-0.886944	2.966840
53	1	0	-4.177875	-1.245938	2.894650
54	1	0	-5.800577	-2.773354	1.883614
55	1	0	-5.428337	-0.719919	-1.863862
56	1	0	-3.786906	0.820199	-0.869333
57	1	0	3.805577	-1.951130	-1.292260
58	1	0	5.864104	-2.788404	-2.368145
59	1	0	8.146911	-1.638983	1.078648
60	1	0	6.102547	-0.821539	2.167426
61	1	0	-0.106814	0.156524	-0.707640
62	1	0	-1.517274	-0.937847	-2.435580
63	1	0	-2.670864	-3.948234	0.401361
64	1	0	-1.236882	-2.854871	2.126362
65	1	0	1.583741	2.850453	-0.807888
66	1	0	1.450276	4.774134	-2.383470
67	1	0	-1.536226	6.595570	0.106942
68	1	0	-1.427123	4.654970	1.657122
69	1	0	-3.767997	0.716354	4.053811
70	1	0	-2.272092	0.549252	4.989789
71	1	0	-2.545445	1.988814	3.978758
72	1	0	5.309090	1.384271	1.388250
73	1	0	3.674295	1.906454	0.913253
74	1	0	4.274566	2.228900	2.554740

$5g_{homo}$-in/in

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.278375	-3.029376	-1.135352
2	6	0	-3.063339	-3.241939	-0.478157
3	6	0	-3.012278	-4.092150	0.628831
4	6	0	-4.174146	-4.680548	1.115351
5	6	0	-5.375676	-4.449153	0.456347
6	6	0	-5.437341	-3.636934	-0.671889
7	7	0	-1.842049	-2.720861	-0.958418
8	6	0	-1.667386	-1.491287	-1.192260
9	6	0	-0.364975	-0.946783	-1.775792
10	6	0	-0.868922	0.380311	-2.434096
11	7	0	-2.036565	0.742358	-1.596685
12	6	0	-2.584228	-0.310184	-0.920758
13	6	0	0.193475	-1.936066	-2.807175
14	8	0	-3.553678	-0.291066	-0.189191
15	6	0	-2.509028	2.068714	-1.433544
16	6	0	-2.769431	2.870820	-2.543416
17	6	0	-3.181890	4.188138	-2.368081
18	6	0	-3.340525	4.682588	-1.078375
19	6	0	-3.096008	3.888713	0.037892
20	6	0	-2.675967	2.577311	-0.143743
21	6	0	0.132116	1.524270	-2.554248

22	35	0	-3.894263	6.478469	-0.836597
23	35	0	-6.959176	-5.274595	1.093109
24	6	0	1.525949	-1.490712	-3.416428
25	6	0	2.427521	-1.125416	-2.283276
26	6	0	1.957695	-0.806955	-1.065823
27	6	0	3.102196	-0.689275	-0.110236
28	7	0	4.242212	-0.872458	-0.871517
29	6	0	3.928187	-1.194848	-2.267285
30	7	0	0.623206	-0.736182	-0.686142
31	6	0	0.245768	0.029636	0.463896
32	6	0	-0.669013	-0.489590	1.383190
33	6	0	-1.142777	0.292846	2.433567
34	6	0	-0.659641	1.585295	2.585425
35	6	0	0.325230	2.088701	1.741647
36	6	0	0.772167	1.307455	0.685300
37	6	0	4.470579	-2.567451	-2.664888
38	6	0	5.562161	-0.772599	-0.389820
39	6	0	5.869470	-1.014099	0.956334
40	6	0	7.181974	-0.912788	1.402254
41	6	0	8.193809	-0.584874	0.508341
42	6	0	7.910036	-0.351432	-0.830707
43	6	0	6.596174	-0.440642	-1.274759
44	8	0	3.054711	-0.482271	1.088329
45	35	0	9.983443	-0.459269	1.121141
46	35	0	-1.402716	2.710754	3.914384
47	1	0	4.343351	-0.422761	-2.929183
48	1	0	-0.565275	-2.085040	-3.580504
49	1	0	0.328267	-2.893365	-2.295386
50	1	0	1.387883	-0.654148	-4.115528
51	1	0	1.948367	-2.313089	-4.003808
52	1	0	-1.225740	0.113556	-3.438984
53	1	0	-2.653410	2.466611	-3.544666
54	1	0	-3.382283	4.821468	-3.224717
55	1	0	-3.213963	4.289520	1.038651
56	1	0	-2.470419	1.946480	0.714553
57	1	0	5.083082	-1.274415	1.650234
58	1	0	7.415223	-1.099170	2.444688
59	1	0	8.703856	-0.094805	-1.523124
60	1	0	6.384290	-0.241082	-2.319347
61	1	0	-1.026800	-1.507326	1.276608
62	1	0	-1.886654	-0.100434	3.117105
63	1	0	0.715667	3.088867	1.891103
64	1	0	1.537098	1.696585	0.021008
65	1	0	-2.057006	-4.281967	1.107875
66	1	0	-4.143170	-5.325389	1.986250
67	1	0	-6.382559	-3.477571	-1.178278
68	1	0	-4.311592	-2.392885	-2.013808
69	1	0	5.557707	-2.606667	-2.558560
70	1	0	4.025366	-3.337433	-2.028332
71	1	0	4.223605	-2.781946	-3.707943
72	1	0	-0.179613	2.230301	-3.326773
73	1	0	0.211475	2.072219	-1.615224
74	1	0	1.120939	1.144847	-2.818594

RCh_{homo}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.632086	0.757789	-0.499303
2	6	0	-3.597432	0.329576	-1.339667
3	6	0	-3.720608	-0.891115	-2.013103
4	6	0	-4.847114	-1.683595	-1.816690
5	6	0	-5.855206	-1.250970	-0.965543
6	6	0	-5.759827	-0.029223	-0.309908
7	7	0	-2.437656	1.130339	-1.472431
8	6	0	-1.189550	0.627309	-1.736168
9	6	0	-0.227696	1.799736	-1.652918
10	6	0	-1.049398	3.007009	-1.457380
11	6	0	-2.502557	2.600814	-1.353517
12	6	0	-0.532708	4.233209	-1.363419
13	7	0	1.043809	1.841373	-1.731102
14	6	0	1.933483	0.764503	-1.894265
15	6	0	1.843446	-0.473140	-1.243375

16	6	0	2.847599	-1.421238	-1.391967
17	6	0	3.939545	-1.140215	-2.205157
18	6	0	4.052980	0.078642	-2.865031
19	6	0	3.060769	1.033299	-2.684225
20	8	0	-0.909524	-0.534223	-1.975238
21	6	0	-3.438751	3.178515	-2.438991
22	35	0	5.340557	-2.404016	-2.340688
23	35	0	-7.377865	-2.338958	-0.690468
24	6	0	0.532360	4.230597	1.367914
25	6	0	1.049261	3.004380	1.460488
26	6	0	0.227744	1.796717	1.654422
27	6	0	1.189779	0.624406	1.736809
28	7	0	2.437871	1.127965	1.474006
29	6	0	2.502524	2.598571	1.356594
30	7	0	-1.043791	1.837986	1.732082
31	6	0	-1.933441	0.760956	1.894344
32	6	0	-1.843508	-0.476265	1.242626
33	6	0	-2.847863	-1.424284	1.390535
34	6	0	-3.939807	-1.143690	2.203860
35	6	0	-4.053052	0.074686	2.864649
36	6	0	-3.060700	1.029306	2.684510
37	35	0	-5.341103	-2.407289	2.338293
38	6	0	3.438382	3.175335	2.442850
39	6	0	3.597781	0.327554	1.340378
40	6	0	4.632411	0.756886	0.500551
41	6	0	5.760214	-0.029804	0.310220
42	6	0	5.855683	-1.252340	0.964371
43	6	0	4.847627	-1.686084	1.814987
44	6	0	3.721052	-0.893928	2.012346
45	8	0	0.909831	-0.537445	1.974403
46	35	0	7.378371	-2.339911	0.687837
47	1	0	-2.879246	2.867915	-0.357574
48	1	0	1.134781	5.110866	1.174280
49	1	0	-0.540061	4.359548	1.478889
50	1	0	0.539663	4.362497	-1.474487
51	1	0	-1.135254	5.113120	-1.168546
52	1	0	2.879409	2.866744	0.361014
53	1	0	4.552099	1.694084	-0.039130
54	1	0	6.548701	0.295540	-0.359652
55	1	0	4.939102	-2.637099	2.327645
56	1	0	2.933897	-1.233080	2.670328
57	1	0	-2.933445	-1.229405	-2.671515
58	1	0	-4.938524	-2.633988	-2.330511
59	1	0	-6.548342	0.295257	0.360352
60	1	0	-4.551851	1.694359	0.041480
61	1	0	1.005074	-0.692617	-0.595463
62	1	0	2.791201	-2.364370	-0.859624
63	1	0	4.918281	0.287578	-3.484288
64	1	0	3.140932	2.006279	-3.158567
65	1	0	-3.140725	2.001971	3.159523
66	1	0	-4.918331	0.283322	3.484039
67	1	0	-2.791593	-2.367049	0.857529
68	1	0	-1.005308	-0.695704	0.594454
69	1	0	-4.420965	2.724291	-2.258402
70	6	0	-3.602021	4.692893	-2.311100
71	6	0	-2.984834	2.788605	-3.844897
72	1	0	4.420702	2.721441	2.262006
73	6	0	3.601456	4.689867	2.316526
74	6	0	2.984228	2.783933	3.848264
75	1	0	-3.668782	3.206505	-4.589239
76	1	0	-1.982505	3.180327	-4.052643
77	1	0	-2.967312	1.702410	-3.979188
78	1	0	-4.448186	5.025782	-2.918770
79	1	0	-3.789869	4.998023	-1.275570
80	1	0	-2.713192	5.218577	-2.672404
81	1	0	3.667928	3.201221	4.593177
82	1	0	1.981777	3.175254	4.056173
83	1	0	2.966885	1.697602	3.981463
84	1	0	4.447522	5.022247	2.924611
85	1	0	3.789350	4.996094	1.281327
86	1	0	2.712527	5.215061	2.678298

RCh_{hetero}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.272795	1.191179	-2.309197
2	6	0	-4.172193	0.587274	-1.696939
3	6	0	-4.275151	-0.732831	-1.242565
4	6	0	-5.467168	-1.432245	-1.389326
5	6	0	-6.556572	-0.811172	-1.988929
6	6	0	-6.468013	0.495571	-2.452139
7	7	0	-2.962403	1.307991	-1.523001
8	6	0	-1.733385	0.715753	-1.710615
9	6	0	-0.704324	1.831509	-1.641070
10	6	0	-1.468283	3.092089	-1.599859
11	6	0	-2.910717	2.765551	-1.266084
12	6	0	-0.946959	4.280018	-1.905269
13	7	0	0.563375	1.780541	-1.741052
14	6	0	1.322642	0.595285	-1.793255
15	6	0	1.132014	-0.492626	-0.932814
16	6	0	2.004864	-1.571725	-0.963035
17	6	0	3.048075	-1.581364	-1.885554
18	6	0	3.250256	-0.516984	-2.755615
19	6	0	2.404363	0.583491	-2.681595
20	8	0	-1.531492	-0.456418	-1.957218
21	6	0	-3.275319	3.134735	0.192953
22	35	0	4.234231	-3.056479	-1.939377
23	35	0	-8.184019	-1.760140	-2.180519
24	6	0	0.501269	4.127051	0.989825
25	6	0	1.216191	3.016792	1.171922
26	6	0	0.649564	1.769806	1.707353
27	6	0	1.768100	0.745668	1.744534
28	7	0	2.850036	1.337902	1.140689
29	6	0	2.670536	2.772945	0.835804
30	7	0	-0.592356	1.596347	1.921761
31	6	0	-1.164052	0.423188	2.446276
32	6	0	-0.776116	-0.130912	3.671114
33	6	0	-1.458561	-1.221854	4.191813
34	6	0	-2.527065	-1.764175	3.483018
35	6	0	-2.936130	-1.222098	2.270834
36	6	0	-2.262669	-0.114943	1.767653
37	35	0	-3.450321	-3.259114	4.193702
38	6	0	3.688715	3.618279	1.633072
39	6	0	4.006512	0.636293	0.728573
40	6	0	4.810703	1.162258	-0.289689
41	6	0	5.899427	0.446416	-0.774078
42	6	0	6.192744	-0.796697	-0.233815
43	6	0	5.435558	-1.315380	0.809204
44	6	0	4.350845	-0.600251	1.297528
45	8	0	1.680015	-0.397043	2.152949
46	35	0	7.612235	-1.818547	-0.951354
47	1	0	-3.589506	3.283373	-1.952994
48	1	0	0.910721	5.024953	0.540347
49	1	0	-0.543358	4.138784	1.288121
50	1	0	0.109624	4.349964	-2.147667
51	1	0	-1.544137	5.184952	-1.947338
52	1	0	2.809267	2.929868	-0.241241
53	1	0	4.582813	2.119001	-0.743831
54	1	0	6.501000	0.849585	-1.581134
55	1	0	5.680845	-2.283795	1.230684
56	1	0	3.755918	-1.012324	2.098309
57	1	0	-3.420827	-1.215951	-0.785074
58	1	0	-5.546647	-2.453890	-1.034921
59	1	0	-7.321554	0.967249	-2.925590
60	1	0	-5.211247	2.207719	-2.680850
61	1	0	0.313180	-0.487779	-0.220289
62	1	0	1.876920	-2.397135	-0.271651
63	1	0	4.077957	-0.534528	-3.456156
64	1	0	2.563761	1.444666	-3.322983
65	1	0	-2.584679	0.345840	0.838375
66	1	0	-3.780908	-1.644250	1.736472
67	1	0	-1.160224	-1.653738	5.140497
68	1	0	0.061397	0.297344	4.210911
69	1	0	4.680265	3.242546	1.351119
70	6	0	3.623438	5.095625	1.247790
71	6	0	3.522404	3.432481	3.140643

72	6	0	-4.615427	2.554010	0.653109
73	1	0	-2.477795	2.725931	0.829332
74	6	0	-3.306681	4.655986	0.358535
75	1	0	4.491413	5.623988	1.652128
76	1	0	3.619758	5.233935	0.160759
77	1	0	2.728862	5.571483	1.660939
78	1	0	4.270878	4.023338	3.676397
79	1	0	2.532201	3.769966	3.467408
80	1	0	3.648336	2.386220	3.436089
81	1	0	-4.819095	2.890227	1.674341
82	1	0	-5.437386	2.900039	0.015224
83	1	0	-4.628167	1.461407	0.657588
84	1	0	-3.581608	4.911307	1.385965
85	1	0	-2.340590	5.120364	0.147676
86	1	0	-4.054442	5.103408	-0.308100

RCh$_{homo}$-in/in

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.216467	-1.988794	0.540499
2	6	0	-5.006863	-1.291306	0.621498
3	6	0	-5.015089	0.057550	0.995795
4	6	0	-6.216230	0.693373	1.287235
5	6	0	-7.408565	-0.014522	1.198779
6	6	0	-7.418515	-1.353089	0.826090
7	7	0	-3.796433	-1.951915	0.299930
8	6	0	-2.587422	-1.636658	0.865806
9	6	0	-1.573047	-2.593054	0.271230
10	6	0	-2.299087	-3.456229	-0.679364
11	6	0	-3.743430	-3.001467	-0.741875
12	6	0	-1.745131	-4.507290	-1.283575
13	7	0	-0.354100	-2.760573	0.582691
14	6	0	0.400179	-1.952842	1.452562
15	6	0	0.572778	-0.581914	1.243924
16	6	0	1.516585	0.128778	1.975996
17	6	0	2.279045	-0.537366	2.928003
18	6	0	2.098120	-1.893846	3.181036
19	6	0	1.169683	-2.600268	2.427595
20	8	0	-2.372354	-0.785563	1.709026
21	6	0	-4.224549	-2.449282	-2.103276
22	35	0	3.646370	0.413586	3.837048
23	35	0	-9.043678	0.858559	1.586618
24	6	0	0.858462	-2.754582	-2.961591
25	6	0	1.604821	-1.758024	-2.489443
26	6	0	1.058784	-0.462265	-2.047672
27	6	0	2.205235	0.305552	-1.411538
28	7	0	3.317978	-0.471783	-1.573660
29	6	0	3.115407	-1.737491	-2.308417
30	7	0	-0.156623	-0.109506	-2.168030
31	6	0	-0.594587	1.201643	-1.888059
32	6	0	-0.102371	2.292403	-2.613983
33	6	0	-0.624047	3.562902	-2.415141
34	6	0	-1.638425	3.744572	-1.479909
35	6	0	-2.143275	2.675195	-0.751824
36	6	0	-1.632341	1.400801	-0.973790
37	35	0	-2.353174	5.478835	-1.204932
38	6	0	3.659018	-2.993680	-1.597811
39	6	0	4.586167	-0.032219	-1.106705
40	6	0	5.649564	0.125366	-1.993478
41	6	0	6.896055	0.519008	-1.517798
42	6	0	7.055293	0.768993	-0.158491
43	6	0	5.995895	0.637673	0.732847
44	6	0	4.757098	0.233545	0.251029
45	8	0	2.145153	1.376845	-0.839817
46	35	0	8.753052	1.301935	0.492891
47	1	0	-4.391373	-3.836749	-0.449682
48	1	0	1.283707	-3.699750	-3.285230
49	1	0	-0.219528	-2.633001	-3.028933
50	1	0	-0.693932	-4.722628	-1.110886
51	1	0	-2.305163	-5.174307	-1.929465
52	1	0	3.603154	-1.657505	-3.290604
53	1	0	5.508321	-0.067006	-3.052694

54	1	0	7.733414	0.636593	-2.196046
55	1	0	6.128167	0.835732	1.790872
56	1	0	3.921248	0.111038	0.931003
57	1	0	-4.085524	0.604923	1.075632
58	1	0	-6.221776	1.738298	1.576182
59	1	0	-8.353736	-1.897538	0.762452
60	1	0	-6.230072	-3.035726	0.257943
61	1	0	-0.011613	-0.069087	0.489190
62	1	0	1.676229	1.182475	1.774887
63	1	0	2.702829	-2.397040	3.927185
64	1	0	1.053176	-3.670497	2.565710
65	1	0	-2.023560	0.557707	-0.414223
66	1	0	-2.933968	2.832942	-0.026667
67	1	0	-0.243929	4.407477	-2.978849
68	1	0	0.688793	2.135871	-3.340415
69	1	0	-5.289230	-2.216820	-1.973631
70	6	0	-3.497841	-1.162165	-2.485235
71	6	0	-4.113214	-3.499975	-3.207526
72	6	0	5.187709	-3.098408	-1.589855
73	6	0	3.085498	-3.145120	-0.192817
74	1	0	3.287864	-3.824142	-2.214276
75	1	0	-4.657730	-3.161689	-4.093348
76	1	0	-3.069643	-3.654600	-3.499367
77	1	0	-4.534385	-4.464241	-2.901316
78	1	0	-3.786075	-0.853461	-3.494722
79	1	0	-3.750898	-0.341427	-1.806821
80	1	0	-2.407980	-1.291914	-2.474107
81	1	0	3.496088	-4.037309	0.290831
82	1	0	3.343564	-2.281387	0.432644
83	1	0	1.996648	-3.238655	-0.215115
84	1	0	5.476815	-4.123670	-1.339319
85	1	0	5.619456	-2.854398	-2.566665
86	1	0	5.637094	-2.437347	-0.843730

TSh_{homo}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.802182	0.771217	-0.525409
2	6	0	-3.727116	0.308161	-1.295047
3	6	0	-3.839290	-0.932127	-1.939468
4	6	0	-4.979979	-1.708712	-1.768718
5	6	0	-6.020642	-1.244119	-0.975871
6	6	0	-5.945133	-0.000742	-0.363318
7	7	0	-2.546838	1.081372	-1.383055
8	6	0	-1.301180	0.560942	-1.651042
9	6	0	-0.319995	1.694569	-1.462938
10	6	0	-1.074430	2.859592	-1.131697
11	6	0	-2.541622	2.530423	-1.099949
12	6	0	-0.417016	4.060138	-0.877296
13	7	0	0.972044	1.740632	-1.515527
14	6	0	1.872238	0.695651	-1.740055
15	6	0	1.766550	-0.613260	-1.240740
16	6	0	2.806801	-1.517674	-1.408403
17	6	0	3.946358	-1.132870	-2.108444
18	6	0	4.068494	0.147096	-2.638006
19	6	0	3.045633	1.060145	-2.422926
20	8	0	-1.041457	-0.585915	-1.970874
21	6	0	-3.411724	3.281642	-2.136952
22	35	0	5.389235	-2.344643	-2.273932
23	35	0	-7.549202	-2.325303	-0.704628
24	6	0	0.417016	4.060138	0.877293
25	6	0	1.074430	2.859593	1.131696
26	6	0	0.319995	1.694570	1.462937
27	6	0	1.301180	0.560943	1.651041
28	7	0	2.546838	1.081373	1.383054
29	6	0	2.541622	2.530424	1.099948
30	7	0	-0.972043	1.740633	1.515526
31	6	0	-1.872238	0.695652	1.740054
32	6	0	-1.766550	-0.613260	1.240740
33	6	0	-2.806801	-1.517673	1.408404
34	6	0	-3.946358	-1.132868	2.108444
35	6	0	-4.068494	0.147098	2.638005

36	6	0	-3.045634	1.060146	2.422924
37	35	0	-5.389236	-2.344641	2.273934
38	6	0	3.411724	3.281643	2.136952
39	6	0	3.727116	0.308162	1.295046
40	6	0	4.802182	0.771218	0.525408
41	6	0	5.945133	-0.000742	0.363317
42	6	0	6.020643	-1.244118	0.975872
43	6	0	4.979980	-1.708710	1.768719
44	6	0	3.839290	-0.932125	1.939468
45	8	0	1.041458	-0.585914	1.970873
46	35	0	7.549202	-2.325301	0.704629
47	1	0	-2.935895	2.707086	-0.088899
48	1	0	0.995896	4.969066	0.752997
49	1	0	-0.531074	4.170298	1.398157
50	1	0	0.531074	4.170297	-1.398159
51	1	0	-0.995896	4.969066	-0.753001
52	1	0	2.935895	2.707087	0.088899
53	1	0	4.747164	1.724815	0.013800
54	1	0	6.760617	0.354753	-0.257048
55	1	0	5.054228	-2.675474	2.254077
56	1	0	3.029287	-1.299586	2.551438
57	1	0	-3.029286	-1.299588	-2.551437
58	1	0	-5.054227	-2.675476	-2.254075
59	1	0	-6.760617	0.354753	0.257046
60	1	0	-4.747164	1.724814	-0.013802
61	1	0	0.883969	-0.917297	-0.694463
62	1	0	2.738648	-2.513824	-0.985321
63	1	0	4.967088	0.434308	-3.173079
64	1	0	3.131419	2.078916	-2.788482
65	1	0	-3.131419	2.078918	2.788480
66	1	0	-4.967088	0.434310	3.173078
67	1	0	-2.738649	-2.513823	0.985323
68	1	0	-0.883969	-0.917298	0.694464
69	1	0	-4.412590	2.839344	-2.062884
70	6	0	-3.539817	4.768310	-1.804670
71	6	0	-2.908487	3.073439	-3.564265
72	1	0	4.412591	2.839347	2.062881
73	6	0	3.539813	4.768311	1.804671
74	6	0	2.908489	3.073437	3.564265
75	1	0	-3.568543	3.582805	-4.272394
76	1	0	-1.900569	3.485651	-3.687440
77	1	0	-2.882535	2.012723	-3.832570
78	1	0	-4.362536	5.207024	-2.376313
79	1	0	-3.742788	4.933527	-0.740572
80	1	0	-2.631477	5.316197	-2.073323
81	1	0	3.568544	3.582803	4.272394
82	1	0	1.900570	3.485645	3.687441
83	1	0	2.882540	2.012720	3.832568
84	1	0	4.362532	5.207026	2.376314
85	1	0	3.742783	4.933531	0.740574
86	1	0	2.631473	5.316196	2.073327

TSh_{hetero}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.169941	0.221721	-2.648470
2	6	0	-4.195217	-0.135204	-1.714963
3	6	0	-4.417998	-1.222539	-0.863948
4	6	0	-5.608134	-1.936193	-0.938782
5	6	0	-6.575681	-1.556238	-1.861963
6	6	0	-6.366633	-0.482942	-2.719149
7	7	0	-2.981617	0.593521	-1.619850
8	6	0	-1.765638	-0.063780	-1.588751
9	6	0	-0.715727	0.997190	-1.813928
10	6	0	-1.394994	2.228335	-2.021405
11	6	0	-2.882798	2.054160	-1.818851
12	6	0	-0.655534	3.363744	-2.343413
13	7	0	0.577074	0.928168	-1.909681
14	6	0	1.347647	-0.211142	-1.650778
15	6	0	1.132330	-1.101924	-0.586092
16	6	0	2.042263	-2.116847	-0.328487
17	6	0	3.154424	-2.267968	-1.154826

18	6	0	3.378510	-1.415205	-2.228136
19	6	0	2.486691	-0.374372	-2.452723
20	8	0	-1.610309	-1.263395	-1.478086
21	6	0	-3.476911	2.897157	-0.657202
22	35	0	4.423352	-3.621215	-0.778653
23	35	0	-8.205489	-2.517860	-1.952197
24	6	0	0.221669	4.034329	-0.776082
25	6	0	1.042786	3.065941	-0.198144
26	6	0	0.541283	2.158844	0.789893
27	6	0	1.697213	1.277910	1.220484
28	7	0	2.780792	1.658918	0.459120
29	6	0	2.514701	2.830614	-0.399087
30	7	0	-0.707665	2.081140	1.097109
31	6	0	-1.218012	1.252089	2.108065
32	6	0	-0.720890	1.267567	3.419117
33	6	0	-1.336300	0.523260	4.415097
34	6	0	-2.453575	-0.247366	4.103928
35	6	0	-2.973476	-0.268788	2.816423
36	6	0	-2.363789	0.497057	1.828832
37	35	0	-3.288675	-1.269532	5.465715
38	6	0	3.435853	4.010709	0.006229
39	6	0	3.978441	0.915918	0.342844
40	6	0	4.853328	1.164726	-0.724737
41	6	0	5.980235	0.375812	-0.921117
42	6	0	6.245747	-0.666190	-0.044441
43	6	0	5.425163	-0.893586	1.052066
44	6	0	4.301062	-0.103323	1.253423
45	8	0	1.647167	0.377590	2.036520
46	35	0	7.715138	-1.813868	-0.363554
47	1	0	-3.408780	2.325972	-2.745323
48	1	0	0.686348	4.874960	-1.281645
49	1	0	-0.664902	4.279911	-0.196324
50	1	0	0.273676	3.150941	-2.868209
51	1	0	-1.173036	4.261205	-2.667945
52	1	0	2.694626	2.551923	-1.447628
53	1	0	4.651132	1.949246	-1.444022
54	1	0	6.632496	0.561029	-1.767340
55	1	0	5.646547	-1.701802	1.740227
56	1	0	3.657894	-0.299098	2.097094
57	1	0	-3.656916	-1.512558	-0.149172
58	1	0	-5.783677	-2.777570	-0.277998
59	1	0	-7.125807	-0.202690	-3.440568
60	1	0	-5.006179	1.051574	-3.327244
61	1	0	0.276021	-0.971536	0.065900
62	1	0	1.898145	-2.780021	0.517242
63	1	0	4.257940	-1.539352	-2.850348
64	1	0	2.656761	0.332412	-3.259455
65	1	0	-2.772272	0.512891	0.823673
66	1	0	-3.852051	-0.862885	2.588312
67	1	0	-0.950124	0.537484	5.428263
68	1	0	0.149970	1.870551	3.652542
69	1	0	4.441992	3.584014	0.095043
70	6	0	3.494998	5.092161	-1.072054
71	6	0	3.058544	4.591996	1.368027
72	6	0	-4.867409	2.438039	-0.211059
73	1	0	-2.786887	2.799142	0.187717
74	6	0	-3.554460	4.371783	-1.066427
75	1	0	4.306515	5.791823	-0.852293
76	1	0	3.677519	4.664777	-2.064145
77	1	0	2.571436	5.677392	-1.114342
78	1	0	3.807613	5.323468	1.684459
79	1	0	2.088465	5.098849	1.326441
80	1	0	3.006579	3.812937	2.136045
81	1	0	-5.220218	3.104087	0.582373
82	1	0	-5.590222	2.483452	-1.033648
83	1	0	-4.870667	1.420500	0.187275
84	1	0	-4.026807	4.951104	-0.268060
85	1	0	-2.575618	4.818031	-1.252663
86	1	0	-4.162454	4.493954	-1.970933

TSh_{homo}-in/in

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-5.664157	-2.012613	1.183350
2	6	0	-4.630694	-1.112424	0.907095
3	6	0	-4.902905	0.260639	0.882403
4	6	0	-6.190303	0.722383	1.127550
5	6	0	-7.207620	-0.187923	1.389391
6	6	0	-6.955231	-1.553546	1.418589
7	7	0	-3.322958	-1.583987	0.646786
8	6	0	-2.194263	-0.953434	1.132073
9	6	0	-1.032018	-1.855532	0.784389
10	6	0	-1.553379	-2.965085	0.061025
11	6	0	-3.062294	-2.893257	0.020452
12	6	0	-0.708286	-3.988821	-0.390215
13	7	0	0.214716	-1.785046	1.130422
14	6	0	0.826912	-0.674188	1.718010
15	6	0	0.648101	0.645529	1.277052
16	6	0	1.442446	1.669576	1.779070
17	6	0	2.398015	1.379336	2.746564
18	6	0	2.560240	0.088537	3.242839
19	6	0	1.787611	-0.933016	2.711884
20	8	0	-2.168267	0.087610	1.757746
21	6	0	-3.820898	-3.084337	-1.311624
22	35	0	3.589841	2.736479	3.318829
23	35	0	-8.963710	0.442835	1.716014
24	6	0	0.148119	-3.498937	-1.978266
25	6	0	1.074032	-2.474055	-1.751264
26	6	0	0.713384	-1.091492	-1.774839
27	6	0	1.965077	-0.312334	-1.416435
28	7	0	2.958971	-1.245744	-1.221221
29	6	0	2.572002	-2.616193	-1.596570
30	7	0	-0.493250	-0.685103	-2.000135
31	6	0	-0.853286	0.663270	-2.132122
32	6	0	-0.149263	1.574070	-2.935150
33	6	0	-0.616011	2.868528	-3.111272
34	6	0	-1.791082	3.266634	-2.479403
35	6	0	-2.518611	2.380130	-1.696136
36	6	0	-2.056300	1.078276	-1.544803
37	35	0	-2.417736	5.041097	-2.708165
38	6	0	3.061015	-3.766883	-0.684580
39	6	0	4.272983	-0.821590	-0.902879
40	6	0	5.374698	-1.223531	-1.654897
41	6	0	6.649816	-0.782977	-1.308846
42	6	0	6.802606	0.077750	-0.228056
43	6	0	5.708146	0.506222	0.517025
44	6	0	4.442985	0.048008	0.177140
45	8	0	2.088550	0.890643	-1.304362
46	35	0	8.537703	0.685101	0.234672
47	1	0	-3.419837	-3.683211	0.701941
48	1	0	0.548720	-4.476700	-2.240110
49	1	0	-0.720307	-3.203167	-2.561001
50	1	0	0.186538	-4.123469	0.213705
51	1	0	-1.171640	-4.916458	-0.713361
52	1	0	2.966231	-2.824558	-2.606576
53	1	0	5.243647	-1.879568	-2.510045
54	1	0	7.514051	-1.096511	-1.883255
55	1	0	5.831490	1.185979	1.353624
56	1	0	3.575152	0.366023	0.742883
57	1	0	-4.104588	0.967367	0.694075
58	1	0	-6.400306	1.785828	1.110151
59	1	0	-7.754649	-2.254094	1.631460
60	1	0	-5.468199	-3.078706	1.227345
61	1	0	-0.079473	0.863545	0.502203
62	1	0	1.340781	2.677829	1.393988
63	1	0	3.307137	-0.116729	4.001453
64	1	0	1.919536	-1.951830	3.060516
65	1	0	-2.627138	0.361458	-0.966527
66	1	0	-3.442116	2.697012	-1.223644
67	1	0	-0.069194	3.567614	-3.734216
68	1	0	0.764106	1.260563	-3.426855
69	1	0	-4.883045	-3.102623	-1.039177
70	6	0	-3.616435	-1.940004	-2.298394
71	6	0	-3.507849	-4.441358	-1.946443
72	6	0	4.440924	-4.308610	-1.074355
73	6	0	3.015044	-3.427487	0.801435

74	1	0	2.346926	-4.582154	-0.871580
75	1	0	-4.246074	-4.659800	-2.722849
76	1	0	-2.524413	-4.447262	-2.426767
77	1	0	-3.541383	-5.256002	-1.214499
78	1	0	-4.104810	-2.180817	-3.247959
79	1	0	-4.062463	-1.012578	-1.925802
80	1	0	-2.553472	-1.753790	-2.484112
81	1	0	3.308783	-4.304110	1.388249
82	1	0	3.713300	-2.616758	1.037481
83	1	0	2.013902	-3.114719	1.101167
84	1	0	4.606027	-5.270170	-0.579019
85	1	0	4.527996	-4.468457	-2.154710
86	1	0	5.241169	-3.634336	-0.758202

5h$_{homo}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.700689	0.616632	-0.963983
2	6	0	-3.534836	0.258300	-1.656955
3	6	0	-3.470008	-1.004922	-2.261810
4	6	0	-4.518575	-1.906878	-2.115862
5	6	0	-5.646687	-1.546298	-1.390202
6	6	0	-5.752606	-0.280473	-0.830035
7	7	0	-2.431379	1.138605	-1.691587
8	6	0	-1.112625	0.702403	-1.675977
9	6	0	-0.301425	1.857554	-1.194560
10	6	0	-1.111155	2.893508	-0.933878
11	6	0	-2.538362	2.523024	-1.217571
12	6	0	-0.688595	4.098778	-0.162944
13	7	0	0.982470	1.757557	-0.669341
14	6	0	2.034104	0.987620	-1.257869
15	6	0	2.086216	-0.401704	-1.119340
16	6	0	3.196484	-1.114234	-1.556752
17	6	0	4.262972	-0.425478	-2.122196
18	6	0	4.214124	0.949329	-2.322181
19	6	0	3.087881	1.648781	-1.895647
20	8	0	-0.720188	-0.422478	-1.931416
21	6	0	-3.300120	3.411057	-2.220294
22	35	0	5.844883	-1.377293	-2.539341
23	35	0	-7.053662	-2.790979	-1.153965
24	6	0	0.702773	3.917080	0.489634
25	6	0	1.109330	2.455097	0.666078
26	6	0	0.229652	1.559631	1.516890
27	6	0	1.110375	0.389259	1.925396
28	7	0	2.409578	0.778155	1.673239
29	6	0	2.504300	2.194469	1.256780
30	7	0	-1.015802	1.752956	1.660644
31	6	0	-1.980129	0.769958	1.954730
32	6	0	-1.993690	-0.454596	1.272623
33	6	0	-3.088866	-1.302004	1.367735
34	6	0	-4.170138	-0.929217	2.158164
35	6	0	-4.171414	0.272009	2.859461
36	6	0	-3.082718	1.128675	2.738440
37	35	0	-5.697991	-2.046861	2.203011
38	6	0	2.981082	3.050495	2.452257
39	6	0	3.528290	-0.084314	1.604719
40	6	0	4.766824	0.420586	1.180739
41	6	0	5.830342	-0.432179	0.913012
42	6	0	5.671478	-1.799548	1.085690
43	6	0	4.477429	-2.312854	1.575867
44	6	0	3.410894	-1.462849	1.844530
45	8	0	0.733522	-0.663361	2.403520
46	35	0	7.089278	-2.967235	0.633721
47	1	0	-3.057589	2.529941	-0.246580
48	1	0	1.473139	4.384576	-0.133329
49	1	0	0.706825	4.430616	1.452339
50	1	0	-0.665606	4.988740	-0.803633
51	1	0	-1.442244	4.287050	0.609011
52	1	0	3.242973	2.281605	0.459400
53	1	0	4.922425	1.480979	1.025881
54	1	0	6.769608	-0.030660	0.548951
55	1	0	4.367783	-3.380106	1.734120

56	1	0	2.479156	-1.873594	2.203460
57	1	0	-2.590438	-1.290676	-2.819841
58	1	0	-4.453631	-2.890191	-2.568634
59	1	0	-6.636369	-0.003480	-0.265863
60	1	0	-4.796116	1.586989	-0.491440
61	1	0	1.269046	-0.920220	-0.630201
62	1	0	3.256096	-2.186804	-1.409288
63	1	0	5.049099	1.467227	-2.780464
64	1	0	3.034681	2.726558	-2.023197
65	1	0	-3.084409	2.092379	3.237861
66	1	0	-5.026985	0.549479	3.465168
67	1	0	-3.117543	-2.228539	0.804174
68	1	0	-1.162934	-0.722049	0.627414
69	1	0	-4.218845	2.866118	-2.474609
70	6	0	-3.706393	4.739538	-1.583032
71	6	0	-2.495953	3.620087	-3.501613
72	1	0	3.855104	2.498270	2.824392
73	6	0	3.490370	4.434658	2.038735
74	6	0	1.988235	3.118894	3.615082
75	1	0	-3.101658	4.135587	-4.252457
76	1	0	-1.606228	4.229918	-3.307744
77	1	0	-2.168549	2.664960	-3.924057
78	1	0	-4.339947	5.309181	-2.269052
79	1	0	-4.266823	4.584047	-0.654685
80	1	0	-2.832842	5.357843	-1.352448
81	1	0	2.448976	3.644606	4.456561
82	1	0	1.070806	3.655673	3.354100
83	1	0	1.708899	2.120591	3.966788
84	1	0	4.073578	4.867647	2.856472
85	1	0	4.141951	4.373125	1.159675
86	1	0	2.681096	5.132045	1.811224

$5h_{hetero}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.024933	-0.968339	1.076344
2	6	0	4.893480	-0.991830	0.254775
3	6	0	4.958125	-1.637667	-0.984466
4	6	0	6.137524	-2.248265	-1.395205
5	6	0	7.256107	-2.200968	-0.571787
6	6	0	7.210905	-1.562284	0.661464
7	7	0	3.695653	-0.373402	0.673201
8	6	0	2.459854	-0.979881	0.537702
9	6	0	1.517958	-0.154100	1.352396
10	6	0	2.199208	0.823356	1.971668
11	6	0	3.616375	0.868556	1.455749
12	6	0	1.615148	1.611354	3.097005
13	7	0	0.182293	-0.485117	1.562183
14	6	0	-0.467506	-1.314689	0.583078
15	6	0	-0.622763	-0.895288	-0.741527
16	6	0	-1.332319	-1.675620	-1.644817
17	6	0	-1.874900	-2.885865	-1.214867
18	6	0	-1.684437	-3.343908	0.079787
19	6	0	-0.969765	-2.551495	0.976176
20	8	0	2.229930	-2.010847	-0.066301
21	6	0	3.904407	2.100511	0.555503
22	35	0	-2.940440	-3.904139	-2.403388
23	35	0	8.869160	-3.019958	-1.139873
24	6	0	0.249662	1.020192	3.483742
25	6	0	-0.590261	0.588338	2.275227
26	6	0	-0.919110	1.696909	1.289179
27	6	0	-2.220327	1.308595	0.602888
28	7	0	-2.744479	0.271615	1.334108
29	6	0	-2.011130	0.053139	2.602204
30	7	0	-0.167730	2.683718	1.034733
31	6	0	-0.524009	3.706315	0.128800
32	6	0	-1.627200	4.532121	0.359526
33	6	0	-1.891279	5.596958	-0.491710
34	6	0	-1.049369	5.826998	-1.575092
35	6	0	0.059474	5.022614	-1.810903
36	6	0	0.331721	3.971750	-0.942223
37	35	0	-1.413062	7.276738	-2.742206

38	6	0	-2.818239	0.684995	3.761933
39	6	0	-3.728005	-0.634285	0.873878
40	6	0	-4.167587	-1.672379	1.707341
41	6	0	-4.987547	-2.680281	1.212587
42	6	0	-5.389274	-2.644163	-0.114947
43	6	0	-5.028893	-1.582552	-0.934308
44	6	0	-4.207562	-0.576506	-0.444882
45	8	0	-2.640298	1.787576	-0.432107
46	35	0	-6.404705	-4.067587	-0.834378
47	1	0	4.333802	0.851438	2.287684
48	1	0	0.388589	0.131668	4.109112
49	1	0	-0.298794	1.756860	4.069607
50	1	0	2.284167	1.557455	3.965339
51	1	0	1.501496	2.666886	2.848151
52	1	0	-1.931186	-1.022483	2.779325
53	1	0	-3.851335	-1.736746	2.741627
54	1	0	-5.293042	-3.497186	1.856688
55	1	0	-5.359707	-1.554602	-1.966548
56	1	0	-3.908364	0.229921	-1.096852
57	1	0	4.083365	-1.661350	-1.621485
58	1	0	6.188025	-2.748180	-2.355935
59	1	0	8.088702	-1.536919	1.297220
60	1	0	5.987892	-0.484428	2.046319
61	1	0	-0.206835	0.058889	-1.057758
62	1	0	-1.483037	-1.342676	-2.665744
63	1	0	-2.102465	-4.294782	0.390792
64	1	0	-0.800923	-2.892417	1.993074
65	1	0	1.201689	3.340416	-1.096413
66	1	0	0.709457	5.221447	-2.655649
67	1	0	-2.746567	6.240551	-0.318793
68	1	0	-2.273792	4.338302	1.210308
69	1	0	-3.825474	0.270778	3.620325
70	6	0	-2.363844	0.227288	5.151847
71	6	0	-2.981371	2.205392	3.666183
72	6	0	5.368209	2.162669	0.111105
73	1	0	3.271213	1.965656	-0.332521
74	6	0	3.506911	3.411948	1.237420
75	1	0	-3.153350	0.439359	5.878490
76	1	0	-2.172558	-0.851337	5.172408
77	1	0	-1.461108	0.736448	5.494804
78	1	0	-3.633854	2.551502	4.473171
79	1	0	-2.033980	2.745973	3.757883
80	1	0	-3.451674	2.497007	2.721287
81	1	0	5.536708	3.072102	-0.473687
82	1	0	6.036721	2.196207	0.980334
83	1	0	5.657184	1.310650	-0.507237
84	1	0	3.895086	4.260891	0.666585
85	1	0	2.420979	3.520086	1.296761
86	1	0	3.922543	3.476396	2.250918

5h$_{homo}$-in/in

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.491561	0.805405	0.802705
2	6	0	-5.516983	-0.008501	0.211536
3	6	0	-5.870900	-0.807732	-0.884463
4	6	0	-7.167367	-0.777480	-1.383038
5	6	0	-8.119847	0.037704	-0.783243
6	6	0	-7.791557	0.826565	0.310898
7	7	0	-4.206828	-0.031082	0.728331
8	6	0	-3.073601	-0.283292	-0.023607
9	6	0	-1.926871	-0.076095	0.904581
10	6	0	-2.372612	0.357906	2.092958
11	6	0	-3.878569	0.409994	2.092344
12	6	0	-1.431458	0.780770	3.172411
13	7	0	-0.611227	-0.137735	0.468274
14	6	0	-0.241926	-1.209234	-0.395581
15	6	0	-0.722366	-2.499233	-0.168778
16	6	0	-0.284442	-3.560660	-0.951951
17	6	0	0.654257	-3.322625	-1.950425
18	6	0	1.126869	-2.040901	-2.207859
19	6	0	0.661184	-0.982644	-1.435877

20	8	0	-3.021487	-0.573203	-1.204466
21	6	0	-4.567914	-0.482966	3.151424
22	35	0	1.373599	-4.786895	-2.912104
23	35	0	-9.889536	0.070265	-1.461717
24	6	0	-0.044771	0.217548	2.854684
25	6	0	0.388150	0.455996	1.394319
26	6	0	1.745082	-0.194789	1.168021
27	6	0	2.624129	0.767335	0.401294
28	7	0	1.950342	1.959911	0.378375
29	6	0	0.659283	1.972651	1.097075
30	7	0	2.010672	-1.360953	1.571198
31	6	0	3.261749	-1.978416	1.339041
32	6	0	4.417161	-1.569295	2.006647
33	6	0	5.610027	-2.255593	1.815535
34	6	0	5.638751	-3.343575	0.949685
35	6	0	4.493965	-3.766299	0.284621
36	6	0	3.297019	-3.091924	0.497159
37	35	0	7.270102	-4.274124	0.679649
38	6	0	-0.464275	2.743128	0.361623
39	6	0	2.623218	3.139196	-0.045959
40	6	0	2.808014	4.199820	0.840786
41	6	0	3.477423	5.345815	0.427305
42	6	0	3.976041	5.407542	-0.869521
43	6	0	3.820490	4.348103	-1.756328
44	6	0	3.138485	3.210108	-1.339820
45	8	0	3.706808	0.533201	-0.094518
46	35	0	4.887795	6.967519	-1.437098
47	1	0	-4.210530	1.450513	2.224602
48	1	0	0.709172	0.644286	3.522661
49	1	0	-0.043223	-0.866816	3.008674
50	1	0	-1.407324	1.879140	3.245151
51	1	0	-1.745331	0.416274	4.155074
52	1	0	0.809075	2.461907	2.071322
53	1	0	2.423083	4.137409	1.853983
54	1	0	3.617724	6.178077	1.107444
55	1	0	4.221490	4.412426	-2.761310
56	1	0	3.004581	2.372638	-2.016320
57	1	0	-5.130002	-1.443439	-1.348887
58	1	0	-7.435652	-1.395102	-2.232938
59	1	0	-8.539732	1.458920	0.775219
60	1	0	-6.246687	1.433343	1.652415
61	1	0	-1.415799	-2.676884	0.648793
62	1	0	-0.637983	-4.568219	-0.764044
63	1	0	1.855219	-1.872854	-2.992932
64	1	0	1.016264	0.025468	-1.632035
65	1	0	2.390214	-3.415777	-0.003635
66	1	0	4.529770	-4.616852	-0.387284
67	1	0	6.512493	-1.942393	2.328333
68	1	0	4.379392	-0.711850	2.670951
69	1	0	-5.598367	-0.625029	2.803041
70	6	0	-3.911797	-1.859506	3.241447
71	6	0	-4.648654	0.211999	4.510527
72	6	0	-0.424744	4.253179	0.636889
73	6	0	-0.532362	2.491751	-1.147140
74	1	0	-1.395942	2.376365	0.806425
75	1	0	-5.220885	-0.403000	5.211135
76	1	0	-3.661164	0.376788	4.951372
77	1	0	-5.148228	1.183366	4.429051
78	1	0	-4.506653	-2.521649	3.877005
79	1	0	-3.831203	-2.322516	2.251961
80	1	0	-2.905114	-1.794861	3.670342
81	1	0	-1.316438	3.121098	-1.580015
82	1	0	0.410397	2.765600	-1.633554
83	1	0	-0.768834	1.453719	-1.387569
84	1	0	-1.379502	4.698720	0.341645
85	1	0	-0.268202	4.469476	1.699863
86	1	0	0.361711	4.753416	0.065612