Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting information

Role of Cations and Confinement in Asymmetric Photochemistry: Enantio and Diastereoselective Photocyclization of Tropolone Derivatives within Zeolites

Abraham Joy, Lakshmi S. Kaanumalle and V. Ramamurthy*

Department of Chemistry, University of Miami, Coral Gables, FL 33124

Contents:

1. Synthesis of tropolone alkyl ethers

Materials: NaY zeolite was obtained from Zeolyst International, The Netherlands. Monovalent cation exchanged zeolites (LiY, KY, RbY and CsY) were prepared by stirring 10 g of NaY with 100 ml of a 10 % solution of the corresponding metal nitrate in water for 12 h with continuous refluxing. The zeolite was filtered and washed thoroughly with distilled water. This procedure was repeated at least three times. Subsequently, the zeolite was dried at 120 °C for about 3h to obtain the cation exchanged zeolite. Tropolone, iodomethane, (2-bromo ethyl) benzene, Bromo methyl acetate and (S)-(+)-1-bromo-2-methylbutane obtained from Aldrich, were used without further purification

A General Methods for the Synthesis of Tropolone Alkyl Ethers (**1a, 1b** and **4**).[43] To a solution of tropolone (1.22 g, 10 mmol), anhydrous potassium carbonate (4.15 g, 30 mmol) and dicyclohexyl-18-crown-6 (375 mg, 1 mmol) in dry acetonitrile (50 ml) iodo/ bromo alkane (50 mmol) was added. The suspension was heated to reflux and stirred vigorously for 12 h at which time the reaction was complete. The suspension was filtered, the filtrate evaporated and the residue dissolved in methylene chloride. This solution was washed with 2N potassium carbonate to remove any unreacted tropolone, dried with $MgSO_4$ and the solvent evaporated to give an oil which was purified by column chromatography (10% isopropanol–hexane) to give tropolone ethers in 70% yield.

The syntheses of tropolone alkyl ethers were also carried out using NaY instead of the dicyclohexyl-18-crown-6. The role of NaY in this reaction is to complex the potassium ions into its cavities thereby freeing the tropolone anion to undergo the reaction. Typical procedure consisted of the following. To a stirred solution of tropolone

(1.22 g, 10 mmol) and anhydrous potassium carbonate (4.15 g, 30 mmol in dry acetonitrile (50 ml) was added NaY (1.5 g, activated at 500 °C). Iodoalkane (50 mmol) was added to the reaction mixture and the reaction was heated to reflux and stirred vigorously for 12 h. Rest was the same as above. Spectral data of the product tropolone alkyl ethers are provided below.

2-Methoxy-cyclohepta-2,4,6-trienone (*Tropolone methyl ether***1a**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.22 (1H, m), 7.11 – 7.05 (1H, t), 7.03 – 7.00 (1H, d), 6.90 – 6.87 (2H, m), 3.86 (3H, s).

LRMS: (EI) m/e (relative intensity), 137 (10), 136 (M^+, 62), 107 (58), 105 (102), 93 (18), 79 (44), 78 (122), 65 (164), 63 (54), 39 (160), 38 (42)

2-Phenethyloxy-cyclohepta-2,4,6-trienone (*Tropolone ethyl phenyl ether* **1b**)

^{1}H NMR (400 MHz, acetone-D_6) δ 7.40 – 7.38 (2H, m), 7.31 – 7.20 (4H, m), 7.07 – 6.99 (2H, m), 6.91 – 6.82 (2H, m), 4.24 – 4.20 (2H, t), 3.14 – 3.10 (2H, t)

^{13}C NMR (100 MHz, acetone-D_6) δ 182.2, 164.3, 138.1, 136.6, 135.4, 132.9, 128.6, 126.8, 125.5, 124.3, 113.5, 70.8, 37.7

LRMS: (EI) m/e (relative intensity), 226 (M+, 3), 208 (2), 135 (10), 122 (40), 105 (110), 104 (42), 94 (10), 79 (36), 77 (57), 65 (28), 51 (38), 39 (60).

2-(2-Methyl-butoxy)-cyclohepta-2,4,6-trienone *((S)-Tropolone-2-methylbutyl ether* **4**)

^{1}H NMR (400 MHz, acetone d_6) δ 7.24 – 6.84 (5H, m), 3.89 – 3.81 (2H, m), 1.93 – 1.84 (1H, m), 1.62 – 1.54 (1H, m), 1.33 – 1.22 (1H, m), 1.02 – 1.01 (3H, d), 0.95 – 0.91 (3H,t).

Synthesis of methyl 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetate (tropolone methyl ester **1c***):* Tropolone methyl ester 1c was synthesized following a

procedure reported above for tropolone alkyl ethers. To anhydrous acetonitrile (150 ml) taken in a dried 250 mL round-bottomed flask tropolone (6.12 g, 50 mmol) and potassium carbonate (20.75 g, 150 mmol) were added. The mixture was vigorously stirred for 30 min. at 60°C until a fine yellow precipitate formed. To the refluxing solution, 300 mg of NaY zeolite activated at 500°C was added and the contents were stirred for additional 20 min. Then methyl bromoacetate (27.7 ml, 250 mmol) was carefully syringed into the reaction mixture. After stirring for 12 h at 60°C temperature, the reaction solution turned reddish brown. A clear solution was obtained after suction filtration. The solvent was removed by rotary evaporation. The residue was dissolved in methylene chloride and washed three times with 15 mL of 0.2 M sodium hydrogen carbonate, the organic layer was dried with anhydrous magnesium sulfate and the solvent was removed *in vacuo*. The viscous dark brown residue was purified by flash chromatography (hexane–ethyl acetate 3:1) to give pure reddish brown oil (8.42 g, 81%). The spectra data of the product are given below.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.14–7.24 (m, 2H), 6.97 (t, 1H, J = 9.8 Hz), 6.86 (m, 1H), 6.75 (d, 1H, J = 9.8 Hz), 4.80 (s, 2H), 3.73 (s, 3H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 180.4, 168.2, 163.4, 138.1, 136.5, 132.2, 129.5, 116.7, 65.7 , 52.3.

Synthesis of amide derivatives of 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetic acid: The chiral amides **7a-m** were synthesized by coupling the tropolone acetic acid and the corresponding amines (Scheme 4). The first step in this procedure is the synthesis of 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetic acid (tropolone acetic acid) which was carried out as described below.

Synthesis of 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetic acid (tropolone acetic acid): Methanol (40 mL), barium hydroxide octahydrate (1.10 g) and methyl 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetate (the methyl ester 1c) (6.00 g, 28.8 mmol) were taken in a 100 mL round bottomed flask. Although the reaction mixture became cloudy and viscous after stirring for 5 min at room temperature the stirring was continued for 2 h. At this stage HCl (2 M) was added to neutralize the base and the reaction mixture turned clear. The reaction mixture was concentrated by rotary evaporation to remove most of the solvent (5 mL of viscous liquid were left), and 20 mL of methylene chloride was added to the residue. The white solid that resulted was filtered and washed with three 5 mL portions of diethyl ether. The product was dried under vacuum for 24 h. A grayish white solid was obtained (3.2 g, yield 59%). The solid was purified by recrystallization from methanol and acetonitrile to give a white solid (2.96 g; m.p.: 144–146°C).

*Synthesis of amide derivatives of 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetic acid (*7a-m*):* 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetic acid (0.28 mmol), 40 mL of dichloromethane, 0.28 mmol of 1-[3-(dimethylamino) propyl]-3-ethylcarbodiimide hydrochloride and 0.33 mmol of the amine/amino alcohol/amino acid methyl ester to be coupled were stirred together for six hours under nitrogen atmosphere in a 50 mL round bottomed flask. Following stirring the reaction mixture was concentrated and purified by column chromatography using (methanol/chloroform eluent). Products were characterized by ^{1}H and ^{13}C-NMR and GC-MS.

2. Characterization of tropolone ether derivatives

*S(+)-2-methyl-2-butylamide of 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetic acid (***7a***):* ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88-0.91 (dd, 6H), 1.10-1.12 (d, 3H), 1.70-1.75 (m, 1H), 3.85-3.91 (m, 1H), 4.50 (s, 2H), 6.72-6.76 (d, 1H), 6.90-6.95 (m, 1H), 7.02-7.07 (m, 1H), 7.20-7.29 (m, 2H), 7.34 (d, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 180.7, 166.4, 163.7, 138, 137.3, 132.7, 129.9, 116.3, 68.7, 50.2, 33.0, 18.7, 17.6.

S(+) methoxy propylamide of 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetic acid (**7b**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.14-1.16 (d, 3H), 3.28 (s, 3H), 3.29-3.36 (m, 2H), 4.13-4.23 (m, 1H), 4.46 (s, 2H), 6.71-6.74 (d, 1H), 6.86-6.92 (m, 1H), 6.98-7.04 (m, 1H), 7.16-7.24 (m, 2H), 7.48 (d, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 180.6, 166.6, 163.7, 138, 137.1, 132.8, 130, 116.3, 75.6, 68.9, 59.2, 45.0, 17.6.

R(+)-1-phenyl ethylamide of 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetic acid (**7c**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.50-1.52 (d, 3H), 4.44-4.56 (dd, 2H), 5.12-5.20 (q, 1H), 6.73-6.76 (d, 1H), 6.90-7.05 (m, 2H), 7.19-7.32 (m, 7H), 7.80 (d, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 181.1, 166.3, 163.9, 143.3, 138, 137.4, 132.7, 130.1, 128.8, 127.5, 126.3, 116.8, 68.9, 48.9, 22.4.

S(-)-1-Naphthyl ethylamide of 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetic acid (**7e**)*:* ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.65–1.67 (d, 3H), 4.45-4.58 (dd, 2H), 5.96-6.03 (q, 1H), 6.67-6.69 (d, 1H), 6.82-6.94 (m, 2H), 7.09-7.23 (m, 2H), 7.39-7.54 (m, 4H), 7.70-7.85 (m, 3H), 8.09-8.11 (d, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 180.7, 166.2, 163.66, 138.5, 138, 137.3, 134, 132.58, 131, 130, 129.1, 128.3, 126.6, 125.9, 125.6, 123.3, 122.8, 116.8, 68.9, 44.7, 21.7.

R (+)-1-Cyclohexyl ethylamide of 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetic acid (**7f**)*:* ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.82-1.66 (m, 11H), 1.03-1.05 (d, 3H), 3.78-3.86 (m, 1H), 4.45 (d, 2H), 6.70-6.74 (m, 1H), 6.85-6.90 (m, 1H), 6.97-7.03 (m, 1H), 7.14-7.20 (m, 2H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 180.7, 166.3, 163.6, 138, 137.3, 132.7, 129.9, 116.3, 68.6, 49.6, 43, 29.2, 29, 26.5, 26.3, 17.9.

L-valine methyl ester amide of 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetic aci d (**7g**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.95–0.97 (d, 6H), 2.18-2.30 (m, 1H), 3.70 (s, 3H), 4.49-4.53 (dd, 1H), 4.55-4.57 (d, 2H), 6.74-6.78 (d, 1H), 6.90-6.96 (m, 1H), 7.00-7.06 (m, 1H), 7.24-7.30 (m, 2H), 7.80 (d, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 180.8, 172, 167.5, 163.6, 138.3, 137.2, 132.5, 130.04, 116.7, 68.8, 57.3, 52.4, 31.0, 19.3, 17.8.

L- Leusine methyl ester amide of 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetic acid (**7h**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88-0.91 (dd, 6H), 1.61-1.68 (m, 3H, ,-CH_2, -CH), 3.67 (s, 3H), 4.55 (s, 2H), 4.57-4.62 (m, 1H), 6.75-6.77 (m, 1H), 6.89-6.94 (m, 1H), 7.00-7.05 (m, 1H), 7.19-7.24 (m, 2H), 7.66-7.68 (d, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 180.7, 172.9, 167.3, 163.6, 138.2, 137.3, 132.6, 130.1, 116.7, 68.7, 52.5, 50.8, 41.0, 25, 23, 21.9.

L-Phenyl alanine methyl ester amide of 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetic acid (**7i**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.04-3.23 (ddd, 2H), 3.70 (s, 3H), 4.44-4.56 (dd, 2H), 4.80-4.86 (m, 1H), 6.64-6.68 (d, 1H), 6.90-6.96 (m, 1H), 6.96-7.02 (m, 1H), 7.14-7.26 (m, 7H), 7.66-7.70 (d, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 180.6, 171.6, 167.3, 163.5, 138.2, 137.2, 136.1, 132.6, 130.0, 129.4, 128.8, 127.2, 116.6, 68.6, 53.5, 52.6, 37.9.

L-proline methyl ester amide of 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetic acid (**7j**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.8-2.2 (m, 6H), 3.65 (s, 3H), 4.45-4.48 (dd, 1H), 4.78-4.92 (dd, 2H), 6.84-6.92 (m, 2H), 6.99-7.06 (m, 1H), 7.18-7.22 (m, 2H).

(-) Norephedrine amide of 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetic acid (**7k**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.05-1.07 (d, 3H), 2.20 (s, 1H), 3.7 (s, 1H), 4.3 (m, 1H), 4.5-4.6 (dd, 2H), 4.9 (d, 1H), 6.77-6.80 (d, 1H), 6.94-6.98 (m, 1H), 7.04-7.10 (m, 1H), 7.19-7.35 (m, 7H), 7.71-7.74 (d, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 180.8, 167.3, 163.7, 141.0, 138.2, 137.5, 132.8, 130.3, 128.3, 127.6, 126.3, 117.3, 76.0, 69, 51.4, 14.

S(+) Amino methoxy phenyl propanol amide of 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetic acid (**7l**):

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.2 (s, 3H), 3.3-3.5 (m, 2H), 4.2-4.3 (m, 1H), 4.3-4.5 (dd, 2H), 4.9 (d, 1H), 6.6-6.7 (d, 1H), 6.8-7.0 (m, 2H), 7.1-7.3 (m, 7H), 7.8 (d, 2H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 180.6, 167.7, 163.3, 141.6, 137.9, 137.5, 133, 129.9, 128.4, 127.6, 126.4, 116.3, 73.1, 72.4, 68.3, 59.2, 55.

D-valinol amide of 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetic acid (**7m**): ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.91-0.95 (dd, 6H), 1.90-1.98 (m, 1H), 3.64-3.73

(m, 2H), 3.76-3.82 (m, 1H), 4.53-4.54 (d, 2H), 6.79-6.81 (d, 1H), 6.92-6.96 (m, 1H), 7.03-7.08 (m, 1H), 7.20-7.30 (m, 2H), 7.70-7.72 (d, 1H).

^{13}C NMR (75 MHz, $CDCl_3$): δ 180.9, 168.1, 163.9, 138.2, 137.5, 133, 130.2, 117.1, 69, 63.7, 57.5, 29.2, 19.69, 18.86.

3. Characterisation of photoproducts

Characterisation of Photoproducts by ^{1}H NMR:

Product ***2a*** from tropolone methyl ether

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.68 (1H, m), 5.99 – 5.98 (1H, d), 5.29 (1H, s), 5.00 (1H, m), 3.63 – 3.58 (1H, m), 3.59 (3H, s)

Product ***2b*** from tropolone ethyl phenyl ether

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.59 (1H, m), 7.32 – 7.20 (5H, m), 6.76 – 6.75 (1H, m), 6.35 – 6.34 (1H, d), 6.14 – 6.12 (1H, d), 3.85 – 3.80 (2H, m), 3.76 – 3.4 (1H, m), 2.99 – 2.93 (2H, m)

^{13}C NMR (100 MHz, $CDCl_3$) δ 204.7, 160.5, 146.1, 138.5, 136.2, 133.8, 129.6, 128.6, 126.3, 85.7, 67.3, 54.5, 36.7.

Product **2c** from methyl 2-((1E,3Z,5Z)-7-oxocyclohepta-1,3,5-trienyloxy)acetate (tropolone methyl ester

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.70 (s, 3H), 3.90-3.92 (m, 1H), 4.18-4.30 (m, 2H), 6.10-6.12 (d, 1H), 6.34-6.36 (m, 1H), 6.80-6.82 (m, 1H), 7.60-7.62 (m, 1H).

Photoproduct **8a**:

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88-0.91 (dd, 6H), 1.10-1.12 (d, 3H), 1.70-1.75 (m, 1H), 3.56-3.60 (m, 1H), 3.9-4.2 (m, 3H), 6.13-6.15 (d, 1H), 6.29-6.30 (m, 1H), 6.81-6.83 (m, 1H), 7.62-7.64 (m, 1H).

Photoproduct **8b**:

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.14-1.16 (d, 3H), 3.28 (s, 3H), 3.29-3.36 (m, 2H), 4.16-4.24 (m, 1H), 3.80-3.82 (m, 1H), 4.0-4.10 (m, 2H), 6.10-6.12 (d, 1H), 6.24-6.30 (m, 1H), 6.78-6.80 (m, 1H), 7.60-7.64 (m, 1H).

Photoproduct **8c**:

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.50-1.53 (d, 3H), 3.80-3.82 (dd, 1H), 4.05-4.25 (m, 2H), 5.12-5.20 (q, 1H), 6.16-6.18 (d, 1H), 6.30-6.32 (m, 1H), 6.81-6.83 (m, 1H), 7.33-7.35 (m, 5H), 7.60-7.62 (m, 1H).

Photoproduct **8e**:

^{1}H NMR (400 MHz, $CDCl_3$): δ 1.64-1.68 (d, 3H), 3.72-3.78 (dd, 1H), 4.05-4.13 (m, 2H), 5.94-6.0 (m, 1H), 6.04-6.12 (d, 1H), 6.24-6.26 (m, 1H), 6.68-6.76 (m, 1H), 7.40-7.50 (m, 4H), 7.60-7.62 (m, 1H), 7.78-7.88 (m, 3H), 8.06-8.10 (m, 1H).

Photoproduct **8f**:

^{1}H NMR (400 MHz, $CDCl_3$):): δ 0.82-1.66 (m, 11H), 1.03-1.05 (d, 3H), 3.80-3.98 (m, 2H), 4.08-4.18 (m, 2H), 5.12-5.20 (q, 1H), 6.12-6.16 (d, 1H), 6.24-6.30 (m, 1H), 6.81-6.83 (m, 1H), 7.60-7.64 (m, 1H).

Photoproduct **8g**:

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.95–0.97 (d, 6H), 2.18-2.30 (m, 1H), 3.70 (s, 3H), 3.73-3.78 (m, 1H), 4.08-4.10 (dd, 2H), 4.86-4.94 (m, 1H), 6.14-6.16 (d, 1H), 6.30-6.32 (m, 1H, 6.82-6.84 (m, 1H), 7.62-7.66 (m, 1H).

Photoproduct **8h**:

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.88-0.91 (dd, 6H), 1.61-1.68 (m, 3H, ,-CH_2, -CH), 3.74 (s, 3H), 3.74-3.80 (m, 1H), 4.04-4.3 (m, 2H), 6.10-6.12 (d, 1H), 6.24-6.26 (m, 1H), 6.78-6.80 (m, 1H), 7.62-7.64 (m, 1H).

Photoproduct **8i**:

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.10-3.16 (m, 2H), 3.70 (s, 3H), 3.73-3.78 (m, 1H), 4.05-4.10 (dd, 2H), 4.86-4.94 (m, 1H), 6.09-6.14 (d, 1H), 6.30-6.32 (m,1H), 6.7-6.8 (m, 1H), 7.1-7.26 (m, 5H), 7.56-7.62 (m, 1H).

Photoproduct **8k**:

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.92-0.96 (d, 3H), 3.7 (s, 1H), 3.8-3.82 (m, 1H), 4.3 (m, 1H), 4.0-4.2 (dd, 2H), 4.9 (d, 1H), 6.10-6.12 (d, 1H), 6.24-6.26 (m, 1H), 6.80-6.84 (m, 1H), 7.20-7.36 (m, 5H), 7.60-7.64 (d, 1H).

Photoproduct **8l**:

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.2 (s, 3H), 3.3-3.5 (m, 2H), 3.74-3.78 (m, 1H), 3.98-4.10 (m, 2H), 4.2-4.3 (m, 1H), 4.9 (m, 1H), 6.11-6.13 (m, 1H), 6.04-6.20 (m, 1H), 6.76-6.78 (m, 1H), 7.22-7.36 (m, 5H), 7.58-7.62 (m, 1H).

Photoproduct **8m**:

^{1}H NMR (400 MHz, $CDCl_3$): δ 0.90-0.94 (dd, 6H), 1.88-1.96 (m, 1H), 3.62-3.72 (m, 2H), 3.82-3.84 (m, 1H), 4.10-4.30 (m, 2H), 6.13-6.16 (d, 1H), 6.30-6.36 (m, 1H), 6.84-6.86 (m, 1H), 7.62-7.66 (m, 1H).

4. Coordinates for geometry optimized structures

Conformer I- coordinates (related to Figure 3)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.506071	-0.386025	-0.986276
2	6	0	-3.554637	-1.369314	-0.946286
3	6	0	-2.247306	-1.346082	-0.384774
4	6	0	-4.396316	0.931903	-0.459345
5	6	0	-1.570529	-0.334688	0.256328
6	6	0	-3.351692	1.534293	0.182164
7	6	0	-2.017507	1.067558	0.542048
8	1	0	-5.448924	-0.631395	-1.468646
9	1	0	-3.825159	-2.319185	-1.403228
10	1	0	-1.711643	-2.284734	-0.485158
11	1	0	-5.280143	1.554007	-0.592812
12	1	0	-3.490606	2.566399	0.495373
13	8	0	-1.232429	1.838244	1.100331
14	8	0	-0.326786	-0.496621	0.737702
15	6	0	0.407012	-1.707849	0.552564
16	1	0	-0.111173	-2.532763	1.061549
17	1	0	0.474474	-1.942235	-0.518143
18	6	0	1.796617	-1.493642	1.155600
19	1	0	1.660094	-1.162598	2.192698
20	1	0	2.288322	-2.473324	1.197681
21	6	0	2.670164	-0.516550	0.392112
22	6	0	3.806584	-0.973048	-0.287721
23	6	0	4.621758	-0.090894	-0.999489
24	6	0	4.307440	1.267445	-1.040803
25	6	0	3.175825	1.733513	-0.367460
26	6	0	2.361970	0.852843	0.345856
27	1	0	4.060195	-2.031072	-0.256094
28	1	0	5.500863	-0.465710	-1.517657
29	1	0	4.939772	1.958556	-1.592193
30	1	0	2.922997	2.790298	-0.395233
31	1	0	1.474783	1.223985	0.850482

Conformer II – coordinates (related to Figure 3)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.462677	1.783973	-0.004999
2	6	0	3.128628	2.087428	-0.010604
3	6	0	1.997593	1.222235	-0.009270
4	6	0	5.042776	0.483344	0.003399
5	6	0	1.923222	-0.151224	-0.002674
6	6	0	4.440404	-0.741699	0.007060
7	6	0	3.039190	-1.153995	0.003823
8	1	0	5.158926	2.618957	-0.007040
9	1	0	2.876396	3.146075	-0.016755
10	1	0	1.049177	1.749500	-0.014375
11	1	0	6.131720	0.466407	0.007305
12	1	0	5.090319	-1.613710	0.013408
13	8	0	2.757417	-2.352914	0.007039
14	8	0	0.747130	-0.807009	-0.001646
15	6	0	-0.491781	-0.097018	-0.004525
16	1	0	-0.557084	0.549453	0.881419
17	1	0	-0.558732	0.539646	-0.897430
18	6	0	-1.611448	-1.139206	0.002368
19	1	0	-1.485663	-1.774703	0.885906
20	1	0	-1.489245	-1.783176	-0.875490
21	6	0	-2.976818	-0.484428	0.002061
22	6	0	-3.609224	-0.145227	1.205868
23	6	0	-4.851663	0.490089	1.208135
24	6	0	-5.482579	0.797853	0.001456
25	6	0	-4.863830	0.465110	-1.204859
26	6	0	-3.621326	-0.170167	-1.202041
27	1	0	-3.126855	-0.390049	2.150005
28	1	0	-5.328982	0.739457	2.152224
29	1	0	-6.452136	1.288613	0.001242
30	1	0	-5.350672	0.694974	-2.149039
31	1	0	-3.148460	-0.434472	-2.145715

Structure-1-coordinates (related to Figure 3)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.809473	0.181560	0.309027
2	6	0	-3.972117	1.264043	0.420052
3	6	0	-2.567299	1.337771	0.238029
4	6	0	-4.440303	-1.151810	0.006691
5	6	0	-1.652789	0.354675	-0.066087
6	6	0	-3.194481	-1.688677	-0.200203
7	6	0	-1.879044	-1.100995	-0.187822
8	1	0	-5.868784	0.362042	0.468565
9	1	0	-4.440638	2.213347	0.666660
10	1	0	-2.170274	2.339239	0.360895
11	1	0	-5.264220	-1.859389	-0.053264
12	1	0	-3.144278	-2.757442	-0.392237
13	8	0	-0.882103	-1.857109	-0.304902
14	8	0	-0.328939	0.637660	-0.258087
15	6	0	0.158422	1.993892	-0.181394
16	1	0	-0.491687	2.657530	-0.759985
17	1	0	0.137218	2.311767	0.868070
18	6	0	1.571511	2.046790	-0.770233
19	1	0	1.503715	1.974554	-1.860567
20	1	0	1.969014	3.046285	-0.549033
21	6	0	2.514518	0.974796	-0.258119
22	6	0	2.713895	0.761601	1.117763
23	6	0	3.531380	-0.278551	1.571968
24	6	0	4.173905	-1.122638	0.656887
25	6	0	4.005511	-0.906622	-0.715165
26	6	0	3.179949	0.132859	-1.166033
27	1	0	2.230059	1.411033	1.843239
28	1	0	3.676191	-0.422914	2.638806
29	1	0	4.816033	-1.923884	1.010262
30	1	0	4.520410	-1.536829	-1.434840
31	1	0	3.054685	0.293490	-2.234277
32	11	0	1.196307	-1.376854	-0.065504

Structure-2-coordinates (related to Figure 3)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.333927	-2.157365	-0.001391
2	6	0	2.985882	-2.419913	-0.006344
3	6	0	1.894330	-1.514821	-0.006855
4	6	0	4.954510	-0.884542	0.004145
5	6	0	1.877781	-0.139214	-0.002784
6	6	0	4.388674	0.366076	0.005563
7	6	0	3.015918	0.800125	0.002264
8	1	0	5.000305	-3.015341	-0.001754
9	1	0	2.697705	-3.467896	-0.010341
10	1	0	0.926470	-2.003942	-0.011213
11	1	0	6.042065	-0.898982	0.007638
12	1	0	5.068359	1.214307	0.009948
13	8	0	2.776755	2.036305	0.004076
14	8	0	0.695163	0.555932	-0.003545
15	6	0	-0.578613	-0.136206	-0.004013
16	1	0	-0.648969	-0.764116	-0.898561
17	1	0	-0.646265	-0.769934	0.886621
18	6	0	-1.681091	0.921479	0.001192
19	1	0	-1.568487	1.557336	-0.890178
20	1	0	-1.565322	1.551528	0.896229
21	6	0	-3.058684	0.286513	0.001426
22	6	0	-3.697197	-0.023122	-1.206187
23	6	0	-4.946757	-0.643556	-1.206473
24	6	0	-5.569882	-0.960906	0.001842
25	6	0	-4.940686	-0.654998	1.209973
26	6	0	-3.691139	-0.034570	1.209253
27	1	0	-3.221447	0.229613	-2.151815
28	1	0	-5.435275	-0.872484	-2.149039
29	1	0	-6.544858	-1.439144	0.002021
30	1	0	-5.424466	-0.892832	2.152775
31	1	0	-3.210626	0.209251	2.154813
32	11	0	0.821239	2.890443	-0.001005

Structure-3-coordinates (related to Figure 3)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.848828	1.706192	-0.070265
2	6	0	3.530726	2.048766	0.034514
3	6	0	2.379578	1.205727	0.096840
4	6	0	5.397834	0.390636	-0.145322
5	6	0	2.282506	-0.159675	0.068447
6	6	0	4.769697	-0.819881	-0.135587
7	6	0	3.360108	-1.194156	-0.050210
8	1	0	5.566565	2.521868	-0.098524
9	1	0	3.309410	3.112662	0.081968
10	1	0	1.446140	1.754758	0.188186
11	1	0	6.482712	0.352104	-0.222183
12	1	0	5.395260	-1.706380	-0.205780
13	8	0	3.034134	-2.379962	-0.075038
14	8	0	1.084509	-0.803379	0.145711
15	6	0	-0.129890	-0.096999	0.226313
16	1	0	-0.139174	0.576208	1.096110
17	1	0	-0.275353	0.521123	-0.679399
18	6	0	-1.222240	-1.169688	0.337222
19	1	0	-1.073191	-1.709787	1.280125
20	1	0	-1.061315	-1.897374	-0.463891
21	6	0	-2.635698	-0.633461	0.276450
22	6	0	-3.104877	0.321027	1.204399
23	6	0	-4.435522	0.763870	1.179890
24	6	0	-5.330673	0.262823	0.221333
25	6	0	-4.878901	-0.680435	-0.713664
26	6	0	-3.543842	-1.113806	-0.689344
27	1	0	-2.439575	0.687796	1.981881
28	1	0	-4.780573	1.472898	1.927533
29	1	0	-6.370083	0.578256	0.224613
30	1	0	-5.567547	-1.098371	-1.442998
31	1	0	-3.212686	-1.865824	-1.401167
32	11	0	-3.450504	1.561923	-1.261632

Complex-1-coordinates (related to Figure 4)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.477528	-1.781158	-0.836665
2	6	0	6.338651	-0.470975	-0.454759
3	6	0	5.169199	0.239239	-0.075249
4	6	0	5.447689	-2.748876	-0.948714
5	6	0	3.859280	-0.173834	0.007119
6	6	0	4.101363	-2.623188	-0.724559
7	6	0	3.289173	-1.502629	-0.311700
8	1	0	7.481262	-2.118231	-1.079962
9	1	0	7.248786	0.122947	-0.428408
10	1	0	5.362787	1.272007	0.191651
11	1	0	5.773575	-3.737501	-1.264714
12	1	0	3.490630	-3.508098	-0.884811
13	8	0	2.051382	-1.660558	-0.214750
14	8	0	2.866042	0.671098	0.412979
15	6	0	3.162921	2.047057	0.721675
16	1	0	3.907560	2.087673	1.524450
17	1	0	3.584134	2.532234	-0.167081
18	6	0	1.886892	2.734055	1.184444
19	1	0	1.551417	2.260868	2.116913
20	1	0	2.173225	3.757518	1.464889
21	6	0	0.729396	2.798910	0.196208
22	6	0	0.873818	2.544308	-1.176238
23	6	0	-0.209891	2.688425	-2.050269
24	6	0	-1.456334	3.092089	-1.566981
25	6	0	-1.615002	3.341990	-0.198948
26	6	0	-0.534959	3.188861	0.670334
27	1	0	1.835743	2.245415	-1.582228
28	1	0	-0.070801	2.500522	-3.111184
29	1	0	-2.290013	3.231173	-2.249688
30	1	0	-2.576014	3.670316	0.187053
31	1	0	-0.664724	3.403021	1.729176
32	11	0	0.459689	-0.236411	0.301891
33	6	0	-2.693822	-0.370817	0.484508
34	6	0	-2.200253	-1.533577	1.380300
35	6	0	-4.050277	-0.629660	-0.148611
36	6	0	-4.169643	-1.155668	-1.441117
37	6	0	-5.430118	-1.395177	-1.991974
38	6	0	-6.583142	-1.117415	-1.256584
39	6	0	-6.472036	-0.591433	0.032356
40	6	0	-5.213108	-0.344088	0.578950
41	1	0	-3.274832	-1.373856	-2.016449
42	1	0	-5.509518	-1.800736	-2.996718
43	1	0	-7.562969	-1.304430	-1.686246
44	1	0	-7.364793	-0.364889	0.608254
45	1	0	-5.135142	0.078987	1.578873
46	1	0	-2.782566	0.520463	1.122215
47	8	0	-1.670608	-0.124354	-0.499157
48	1	0	-1.925936	0.659634	-1.014753
49	6	0	-1.946348	-2.831413	0.609417
50	1	0	-1.675949	-3.636544	1.302304
51	1	0	-2.845860	-3.143401	0.073705

52	1	0	-1.137136	-2.721803	-0.120209
53	1	0	-3.008713	-1.715211	2.107475
54	7	0	-0.960261	-1.128824	2.095835
55	1	0	-0.505259	-1.985617	2.410070
56	6	0	-1.199945	-0.293141	3.285436
57	1	0	-1.548539	0.700774	2.987728
58	1	0	-1.945804	-0.723561	3.971158
59	1	0	-0.260024	-0.168188	3.832034

Complex-2-coordinates (related to Figure 4)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.539788	-1.960739	0.411363
2	6	0	-5.514244	-0.684503	-0.092697
3	6	0	-4.403231	0.136291	-0.417039
4	6	0	-4.421500	-2.767137	0.736609
5	6	0	-3.050557	-0.102455	-0.312982
6	6	0	-3.082868	-2.484515	0.644191
7	6	0	-2.369011	-1.311252	0.200651
8	1	0	-6.517387	-2.403661	0.579743
9	1	0	-6.479695	-0.221751	-0.281557
10	1	0	-4.688158	1.104410	-0.812544
11	1	0	-4.659708	-3.756458	1.121370
12	1	0	-2.393713	-3.262400	0.963062
13	8	0	-1.117386	-1.315433	0.247001
14	8	0	-2.127559	0.822694	-0.696087
15	6	0	-2.555854	2.108169	-1.184688
16	1	0	-3.193292	1.970363	-2.065758
17	1	0	-3.143993	2.606908	-0.405729
18	6	0	-1.326710	2.923961	-1.565974
19	1	0	-0.818970	2.430067	-2.403217
20	1	0	-1.700605	3.878037	-1.963821
21	6	0	-0.332417	3.193908	-0.448983
22	6	0	-0.743705	3.617363	0.824939
23	6	0	0.192326	3.942393	1.807237
24	6	0	1.560766	3.853354	1.536550
25	6	0	1.985733	3.427242	0.277838
26	6	0	1.044714	3.095327	-0.703683
27	1	0	-1.801651	3.722113	1.051362
28	1	0	-0.148175	4.282417	2.781097
29	1	0	2.286821	4.128834	2.295966
30	1	0	3.046173	3.371278	0.047667
31	1	0	1.386447	2.799543	-1.693473
32	11	0	0.455414	0.170134	-0.150157
33	6	0	3.426887	-1.890623	-0.669854
34	1	0	3.906870	-2.877976	-0.582803
35	6	0	2.841828	-1.534064	0.691369
36	6	0	2.343087	-2.532810	1.539503
37	6	0	1.796566	-2.211234	2.782745
38	6	0	1.746258	-0.881851	3.207106
39	6	0	2.262196	0.122687	2.384201
40	6	0	2.811261	-0.202600	1.137852
41	1	0	2.394394	-3.574031	1.232379
42	1	0	1.422216	-3.002096	3.426418
43	1	0	1.332523	-0.633345	4.180117
44	1	0	2.256778	1.157614	2.714844
45	1	0	3.248746	0.572383	0.514470
46	6	0	2.399936	-2.042655	-1.823916
47	1	0	3.016230	-2.279434	-2.705532
48	6	0	1.428546	-3.203791	-1.588600
49	1	0	0.846404	-3.396166	-2.497684
50	1	0	1.968437	-4.125846	-1.350838
51	1	0	0.728363	-2.989600	-0.774433

52	7	0	1.622521	-0.802351	-2.096620
53	1	0	0.779358	-1.112425	-2.581947
54	6	0	2.309183	0.140595	-3.007752
55	1	0	3.173130	0.575292	-2.506032
56	1	0	2.660762	-0.346676	-3.929156
57	1	0	1.611966	0.938201	-3.286808
58	8	0	4.385855	-0.929498	-1.107442
59	1	0	5.128827	-0.939088	-0.482797

Complex-3-coordinates (related to Figure 4)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.589837	-1.980556	0.888035
2	6	0	-5.624010	-0.851684	0.108127
3	6	0	-4.556246	-0.030327	-0.337115
4	6	0	-4.442053	-2.585761	1.456261
5	6	0	-3.202026	-0.115735	-0.101559
6	6	0	-3.128105	-2.197178	1.396578
7	6	0	-2.479037	-1.078431	0.757817
8	1	0	-6.540236	-2.464925	1.093776
9	1	0	-6.604626	-0.533740	-0.237012
10	1	0	-4.880543	0.789641	-0.967835
11	1	0	-4.631782	-3.486673	2.035733
12	1	0	-2.409569	-2.812291	1.932420
13	8	0	-1.247838	-0.917223	0.929774
14	8	0	-2.320379	0.762488	-0.655209
15	6	0	-2.792653	1.871123	-1.442531
16	1	0	-3.419106	1.506434	-2.263927
17	1	0	-3.404086	2.521167	-0.804809
18	6	0	-1.588208	2.605705	-2.021872
19	1	0	-1.133906	1.981328	-2.799717
20	1	0	-1.980549	3.492802	-2.538831
21	6	0	-0.517733	3.022336	-1.027222
22	6	0	-0.825966	3.474422	0.267465
23	6	0	0.184148	3.882165	1.143760
24	6	0	1.522699	3.851614	0.741202
25	6	0	1.844586	3.405578	-0.542730
26	6	0	0.832649	2.988689	-1.414499
27	1	0	-1.860123	3.523208	0.597487
28	1	0	-0.077898	4.237153	2.136385
29	1	0	2.304019	4.183878	1.418162
30	1	0	2.879225	3.390820	-0.873372
31	1	0	1.091118	2.660500	-2.419072
32	11	0	0.206370	0.611192	0.292669
33	6	0	3.326111	-0.585997	1.421358
34	1	0	3.737977	-1.515795	1.848202
35	6	0	3.687404	-0.609709	-0.095443
36	1	0	3.550597	0.410348	-0.492542
37	7	0	1.855981	-0.555575	1.610343
38	1	0	1.501314	-1.415702	1.187168
39	6	0	1.438497	-0.594944	3.027850
40	1	0	1.973537	-1.363392	3.606602
41	1	0	1.609148	0.373396	3.505612
42	1	0	0.368021	-0.814177	3.063486
43	8	0	5.038406	-1.032705	-0.251632
44	1	0	5.623508	-0.347645	0.106322
45	6	0	2.818545	-1.550544	-0.904385
46	6	0	1.916844	-1.048338	-1.852414
47	6	0	1.088230	-1.907634	-2.581093
48	6	0	1.158135	-3.284851	-2.369004
49	6	0	2.066105	-3.796287	-1.437230
50	6	0	2.891170	-2.937166	-0.710749
51	1	0	1.900837	0.021914	-2.059401

52	1	0	0.410992	-1.504565	-3.329671
53	1	0	0.524723	-3.958127	-2.939267
54	1	0	2.139535	-4.869349	-1.284563
55	1	0	3.614126	-3.341838	-0.008540
56	6	0	3.997066	0.601057	2.117050
57	1	0	5.073761	0.609209	1.916936
58	1	0	3.572639	1.549602	1.765208
59	1	0	3.886015	0.556978	3.203883

Coordinates related to Figure 5-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.517796	0.806775	0.267784
2	6	0	5.289033	-0.408464	-0.334217
3	6	0	4.058203	-1.071947	-0.544560
4	6	0	4.544621	1.696470	0.782501
5	6	0	2.761393	-0.689474	-0.272275
6	6	0	3.174267	1.599755	0.775689
7	1	0	6.553026	1.122952	0.361570
8	1	0	6.164848	-0.957335	-0.670450
9	1	0	4.125823	-2.056635	-1.000512
10	1	0	4.940479	2.603171	1.234832
11	1	0	2.625517	2.437263	1.200427
12	8	0	1.824980	-1.599460	-0.671148
13	6	0	0.809201	-2.018288	0.230500
14	1	0	0.881711	-3.110906	0.301879
15	1	0	0.958639	-1.601617	1.231430
16	6	0	-0.582327	-1.633134	-0.283923
17	8	0	-0.754758	-1.043356	-1.354552
18	7	0	-1.611076	-1.955607	0.530856
19	1	0	-1.436653	-2.472216	1.384198
20	6	0	-3.002579	-1.575712	0.216859
21	1	0	-3.243310	-2.002329	-0.762902
22	6	0	-3.938357	-2.181813	1.268155
23	1	0	-3.727889	-1.787278	2.268887
24	1	0	-4.976613	-1.939721	1.026655
25	1	0	-3.841266	-3.272681	1.291317
26	6	0	-3.134501	-0.056541	0.110632
27	6	0	-2.708373	0.782488	1.152221
28	6	0	-2.777285	2.173944	1.023920
29	6	0	-3.279785	2.747658	-0.150558
30	6	0	-3.725714	1.918913	-1.187256
31	6	0	-3.652054	0.527728	-1.054322
32	1	0	-2.303880	0.352074	2.064547
33	1	0	-2.446935	2.807643	1.842080
34	1	0	-3.342558	3.827669	-0.247856
35	1	0	-4.134255	2.352989	-2.095524
36	1	0	-3.980909	-0.108817	-1.871764
37	6	0	2.279667	0.595555	0.253514
38	8	0	1.039650	0.825542	0.258667
39	11	0	-0.746950	1.159066	-0.969685

Coordinates related to Figure 5-b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.987502	-0.235224	-0.366670
2	6	0	-5.259144	-1.372414	-0.138595
3	6	0	-3.895291	-1.487064	0.251044
4	6	0	-5.537199	1.113639	-0.283223
5	6	0	-2.940179	-0.523264	0.436162
6	6	0	-4.292720	1.609019	-0.007686
7	1	0	-7.032564	-0.368494	-0.633311
8	1	0	-5.785754	-2.318047	-0.237978
9	1	0	-3.557573	-2.502993	0.446996
10	1	0	-6.300690	1.862968	-0.481372
11	1	0	-4.173981	2.689551	-0.022483
12	8	0	-1.699536	-0.902959	0.885711
13	6	0	-0.857707	-1.735065	0.101080
14	1	0	-0.558860	-2.607040	0.692237
15	1	0	-1.367184	-2.095041	-0.801151
16	6	0	0.416622	-1.001266	-0.325816
17	8	0	1.339880	-1.674508	-0.836534
18	7	0	0.445569	0.313976	-0.117136
19	1	0	-0.423331	0.755529	0.237183
20	6	0	1.512175	1.206907	-0.593882
21	1	0	1.508937	1.179648	-1.691875
22	6	0	1.194960	2.639921	-0.138142
23	1	0	1.222190	2.717675	0.953686
24	1	0	1.932278	3.334164	-0.550727
25	1	0	0.199160	2.938787	-0.477549
26	6	0	2.896607	0.766493	-0.131142
27	6	0	3.126548	0.312242	1.177818
28	6	0	4.397263	-0.122263	1.571188
29	6	0	5.465792	-0.097417	0.663730
30	6	0	5.254957	0.385179	-0.634545
31	6	0	3.978439	0.812172	-1.025607
32	1	0	2.302712	0.281871	1.885746
33	1	0	4.556773	-0.469590	2.588240
34	1	0	6.454541	-0.423455	0.973026
35	1	0	6.081307	0.438105	-1.338120
36	1	0	3.821460	1.177009	-2.038290
37	6	0	-3.031619	0.942941	0.267086
38	8	0	-1.994438	1.627996	0.369970
39	11	0	3.471122	-1.861812	-0.634026

Coordinates related to Figure 6-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.813003	-0.419383	0.350369
2	6	0	5.179749	0.790418	0.207404
3	6	0	3.800171	1.061489	0.015311
4	6	0	5.218111	-1.705975	0.331287
5	6	0	2.735919	0.198954	-0.083655
6	6	0	3.904446	-2.064504	0.161603
7	1	0	6.889690	-0.393657	0.492825
8	1	0	5.809998	1.674937	0.246707
9	1	0	3.569492	2.119010	-0.065519
10	1	0	5.908358	-2.535542	0.466926
11	1	0	3.676686	-3.127264	0.175241
12	8	0	1.455554	0.659822	-0.256231
13	6	0	1.164022	2.062120	-0.357838
14	1	0	1.501324	2.587185	0.546272
15	1	0	1.643514	2.502788	-1.235898
16	6	0	-0.354629	2.215678	-0.523285
17	8	0	-0.810467	3.017486	-1.311979
18	7	0	-1.120885	1.349919	0.252249
19	6	0	2.716273	-1.277239	-0.047755
20	8	0	1.616075	-1.864999	-0.202991
21	6	0	-2.582590	1.603720	0.405389
22	6	0	-2.845010	2.384824	1.698651
23	1	0	-2.840108	2.243108	-0.443015
24	1	0	-3.913059	2.601057	1.802741
25	1	0	-2.530456	1.828352	2.589926
26	1	0	-2.311195	3.340468	1.685529
27	1	0	-0.659829	1.059203	1.112535
28	6	0	-4.282488	-1.517955	-1.297830
29	6	0	-3.435670	-0.243355	-1.159481
30	6	0	-3.407773	0.298507	0.284292
31	6	0	-3.018139	-0.800983	1.294487
32	6	0	-3.877961	-2.066412	1.140801
33	6	0	-3.849733	-2.598608	-0.298013
34	1	0	-2.408361	-0.461450	-1.511913
35	1	0	-3.801918	0.535671	-1.839029
36	1	0	-5.335692	-1.262742	-1.118378
37	1	0	-4.227052	-1.894411	-2.325887
38	1	0	-1.956261	-1.087394	1.164708
39	1	0	-3.091711	-0.421686	2.320412
40	1	0	-3.538683	-2.834652	1.845087
41	1	0	-4.913779	-1.826422	1.416486
42	1	0	-2.828823	-2.942694	-0.542938
43	1	0	-4.491709	-3.481549	-0.390161
44	1	0	-4.441520	0.589854	0.521448
45	11	0	-0.292565	-0.935258	-0.658243

Coordinates related to Figure 6-b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.454083	-1.113578	0.049689
2	6	0	5.241578	0.177419	0.460124
3	6	0	4.024359	0.908210	0.488643
4	6	0	4.482119	-2.038317	-0.421446
5	6	0	2.745148	0.530477	0.166796
6	6	0	3.127020	-1.895699	-0.555017
7	1	0	6.477006	-1.478543	0.086902
8	1	0	6.114846	0.734311	0.789907
9	1	0	4.101898	1.938852	0.826526
10	1	0	4.875157	-3.012532	-0.704480
11	1	0	2.571165	-2.759959	-0.910261
12	8	0	1.785908	1.486353	0.395183
13	6	0	0.965738	1.926027	-0.694338
14	1	0	1.272916	2.938952	-0.972150
15	1	0	1.064745	1.267374	-1.562528
16	6	0	-0.503042	1.980209	-0.264476
17	8	0	-1.172601	3.023033	-0.491954
18	7	0	-0.978610	0.889754	0.308379
19	6	0	2.240401	-0.786361	-0.262002
20	8	0	1.006185	-0.949970	-0.386055
21	6	0	-2.357777	0.710820	0.792196
22	6	0	-2.442478	1.064828	2.284157
23	1	0	-2.965076	1.431168	0.231783
24	1	0	-3.467598	0.934276	2.647500
25	1	0	-1.783819	0.433288	2.887051
26	1	0	-2.148513	2.107191	2.449579
27	1	0	-0.315422	0.104231	0.340088
28	6	0	-3.553602	-2.297669	-1.428978
29	6	0	-2.922355	-0.941064	-1.077940
30	6	0	-2.887848	-0.701783	0.445174
31	6	0	-2.155570	-1.861088	1.154819
32	6	0	-2.795244	-3.216652	0.806590
33	6	0	-2.838662	-3.450614	-0.709908
34	1	0	-1.896496	-0.909418	-1.471479
35	1	0	-3.476889	-0.129036	-1.570842
36	1	0	-4.614406	-2.289634	-1.138852
37	1	0	-3.529122	-2.449712	-2.514923
38	1	0	-1.100550	-1.883544	0.847398
39	1	0	-2.170336	-1.717836	2.241833
40	1	0	-2.241255	-4.023021	1.301883
41	1	0	-3.817878	-3.247730	1.210018
42	1	0	-1.811355	-3.535323	-1.093057
43	1	0	-3.336223	-4.402098	-0.932693
44	1	0	-3.928834	-0.705482	0.804751
45	11	0	-2.265712	4.725420	-0.863137