Diketopyrrolopyrroles disubstituted with alkylated thiophenes: effect of the donor unit size and solubilizing substituents on their redox, photo- and electroluminescence properties

Gabriela Wiosna-Salyga[a]*, Monika Gora[b], Malgorzata Zagorska[c]**, Petr Toman[d], Beata Luszczynska[a], Jiri Pfleger[d], Ireneusz Glowacki[a], Jacek Ulanski[a], Jozef Mieczkowski[b] and Adam Pron[c]***

[a]*Department of Molecular Physics, Lodz University of Technology, Zeromskiego 116, 90-924 Lodz, Poland*
[b]*Faculty of Chemistry, Warsaw University, Pasteura 1, 02-093 Warsaw, Poland*
[c]*Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warsaw, Poland*
[d]*Institute of Macromolecular Chemistry AS CR, Heyrovsky Sq. 2, 162 06 Prague 6, Czech Republic*

* email: gabriela.wiosna-salyga@p.lodz.pl
** email: zagorska@ch.pw.edu.pl
*** email: apron@ch.pw.edu.pl

Content

1. Synthetic procedures and characterization
2. Cyclic voltammetry of n-octyl substituted derivatives of **T1**, **T2** and **T3** compounds.
3. Experimental absorption and emission spectra
4. Calculated molecular geometries include equilibrium cartesian coordinates of all molecules:
a) in vacuum,
b) in DCM (neutral molecule),
c) in DCM (cation-radical),
d) in DCM (anion-radical),
e) in chlorobenzene (neutral molecule).
5. Absorption spectra (40 transitions) of all molecules in chlorobenzene calculated using
a) TD CAM-B3LYP method,
b) TD PBE0 method.

1. Synthetic procedures and characterization

3,6-bis(thiophen-2-yl)-2,5-dihydropyrrolo[3,4-c]-pyrrole-1,4-dione (**1**) was obtained from diethyl succinate ester and 2-thiophene carbonitrile according to the procedure published in [1].
Synthetic route to the derivatives of series **T1** (*Scheme S1*) and synthetic procedures are presented below.
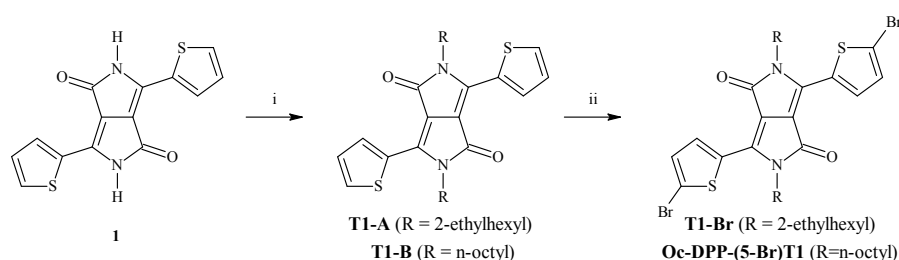
Scheme S1. i. R-Br, K$_2$CO$_3$, DMF, 110 °C, ii. NBS, CHCl$_3$, RT.

The synthetic procedure of **3,6-bis(thiophen-2-yl)-2,5-dioctyl-pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione (T1-B)** was based on the methods published in [2] and [3].

1.500 g (4.994 mmol) of (**1**), 2.070 g (14.982 mmol) of K_2CO_3, 18-crown-6 ether and 70 ml of DMF were added to the double-neck-round-bottom flask under argon and the mixture was heated to 60 °C. Then 2.030 g (10.487 mmol) of n-octyl bromide was injected in one portion and the reaction mixture was stirred at 120 °C for 24 h. After cooling to room temperature, the mixture was poured into 150 ml of water. The water phase was extracted with toluene. The collected organic phases were then dried over $MgSO_4$ and evaporated. The crude product was dissolved in $CHCl_3$ and the pure product was precipitated with MeOH to give 1.200 g (46%) of maroon solid.

^{1}HNMR (500 MHz, $CDCl_3$), δ [ppm]: 8.92 (d, J=3.75 Hz, 2H), 7.63 (d, J= 5.00 Hz, 2H), 7.29 – 7.26 (m, 2H), 4.06 (t, J=8.00 Hz, 4H), 1.74 (quint, J=7.50 Hz, 4H), 1.44 – 1.22 (m, 20 H), 0.87 (t, J=7.00 Hz, 6H).^{13}CNMR (125 MHz, $CDCl_3$), δ [ppm]: 161.36, 140.01, 135.26, 130.66, 129.79, 128.60, 107.69, 42.23, 31.78, 29.96, 29.21, 29.19, 26.88, 22.63, 14.09. MS (TOF - ES$^+$, m/z): calculated for $C_{30}H_{40}N_2O_2S_2$ (M+Na)$^+$: 547.243, found 547.244. Elemental analysis: %C: 68.64 (calc. 68.66), %H: 7.42 (calc. 7.68), %N: 5.38 (calc. 5.34), %S: 12.57 (calc. 12.22).

3,6-bis(thiophen-2-yl)-2,5-di(2-ethylhexyl)-pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione (T1-A) was obtained with 36% yield using an analogous procedure. The synthetic procedures of this compound have been already published in [4], [5] and [6].

^{1}HNMR (400 MHz, $CDCl_3$), δ [ppm]: 8.90 (dd, J_1=3.90 Hz, J_2=1.20 Hz, 2H), 7.63 (dd, J_1= 5.00 Hz, J_2=1.20 Hz, 2H), 7.27 (dd, J_1= 5.00 Hz, J_2=3.90 Hz, 2H), 4.08-3.97 (m, 4H), 1.91-1.80 (m, 2H), 1.44-1.18 (m, 16H), 0.89-0.83 (m, 12H). ^{13}CNMR (100 MHz, $CDCl_3$), δ [ppm]: 161.65, 140.33, 135.27, 130.50, 129.76, 128.37, 107.81, 45.79, 39.02, 30.15, 28.30, 23.47, 23.05, 14.03, 10.45. Elemental analysis calculated for $C_{30}H_{40}N_2O_2S_2$: %C: 68.08 (calc. 68.66), %H: 7.60 (calc. 7.68), %N: 5.15 (calc. 5.34), %S: 12.72 (calc. 12.22).

3,6-bis(5-bromothiophen-2-yl)-2,5-dioctyl-pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione (Oc-DPP-(5-Br)T1) was synthesized according to the method presented in [2] and [7].

1. 000 g (1. 905 mmol) of (**T1-B**) was dissolved in 60 ml of dry $CHCl_3$ in a round-bottom flask. 0.712 g (4.000 mmol) of N-bromosuccinimide was added portion-wise, the reaction was stirred for 8 h at room temperature. Then, the reaction mixture was poured into 50 ml of water, the water phase was separated and extracted with $CHCl_3$. The collected organic phases were washed with water and dried over $MgSO_4$ and the solvent was removed. The crude product was purified by crystallization from CH_2Cl_2 giving 0.640 g (49%) of maroon needles-like crystals.

^{1}HNMR (300 MHz, $CDCl_3$), δ [ppm]: 8.70 (d, J=6.00 Hz, 2H), 7.25 (d, J=4.20 Hz, 2H), 4.00 (t, J=7.80 Hz, 4H), 1.73 (quint, J=7.50 Hz, 4H), 1.48 – 1.20 (m, 20H), 0,90 (t, J=6.60 Hz, 6H). ^{13}CNMR (125 MHz, $CDCl_3$) δ [ppm]: 161.05, 139.00, 135.36, 131.65, 131.11, 119.16, 107.81, 42.30, 31.77, 29.98, 29.16, 26.83, 22.64, 14.11 (4C). MS (TOF - ES$^+$, m/z): calculated for $C_{30}H_{38}Br_2N_2O_2S_2$ (M+Na)$^+$: 705.062, found 705.066.

3,6-bis(5-bromothiophen-2-yl)-2,5-di(2-ethylhexyl)-pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione (T1-Br) was obtained in an analogous procedure with 76% yield. The synthesis of this compound was presented in [8].

^{1}HNMR (400 MHz, $CDCl_3$), δ [ppm]: 8.64 (d, J=4.20 Hz, 2H), 7.22 (d, J=4.20 Hz, 2H), 3.98-3.87 (m, 4H), 1.88-1.78 (m, 2H), 1.42-1.18 (m, 16H), 0,90-0.85 (m, 12H). ^{13}CNMR (125

MHz, CDCl$_3$) δ [ppm]: 161.37, 139.39, 135.40, 131.46, 131.16, 119.03, 107.98, 45.99, 39.09, 30.15, 28.31, 23.55, 23.04, 14.03, 10.46. MS (TOF - ES$^+$, m/z): calculated for C$_{30}$H$_{38}$Br$_2$N$_2$O$_2$S$_2$ (M+Na)$^+$: 705.062, found 705.078.

Scheme S2 presents three synthetic pathways leading to the synthesis of compounds of series **T2** and **T3**.
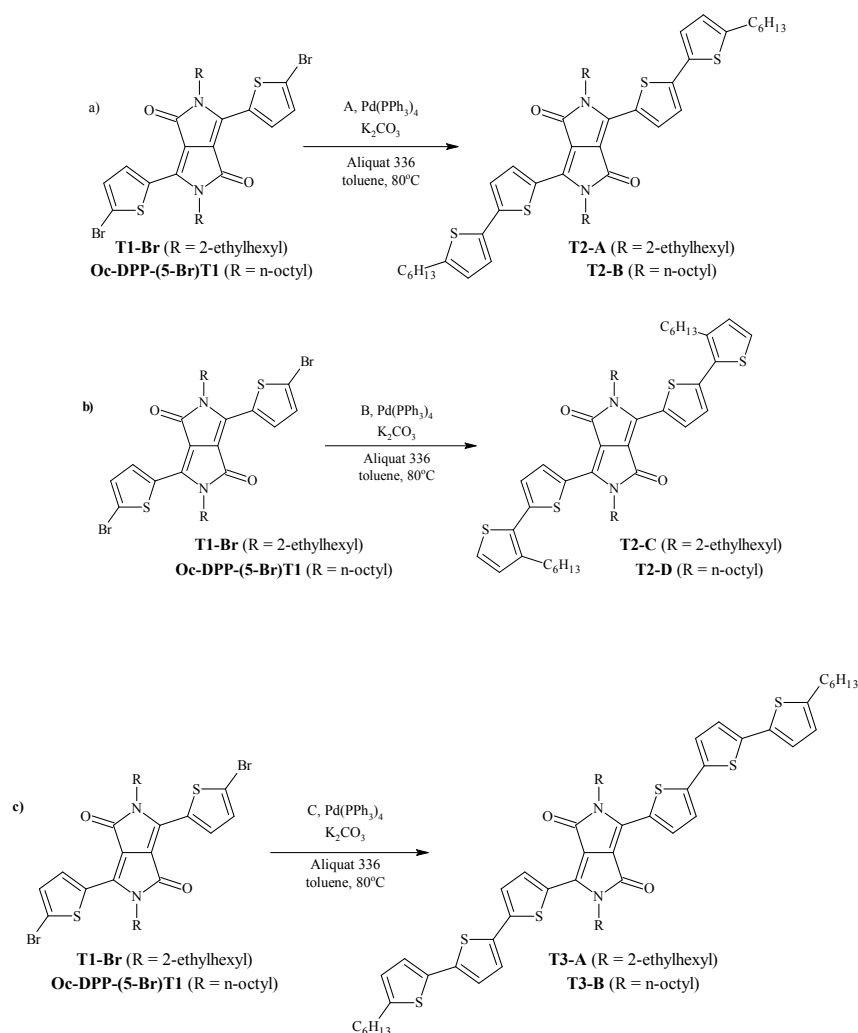
Scheme S2. a) **T2** series (substitution at position 5); A: 5-hexyl-2-thiopheneboronic acid pinacol ester; b) **T2** series (substitution at position 3); B: 3-hexyl-2-thiopheneboronic acid pinacol ester; c) **T3** series; C: 5′-hexyl-2,2′-bithiophene-5-boronic acid pinacol ester.

3,6-bis(5'-hexyl-2,2'-bithiophen-5-yl)-2,5-dioctyl-pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione (T2-B)

A 50 ml round-bottom flask was charged under argon atmosphere with 30 ml of toluene, 500 mg (0.732 mmol) of **(Oc-DPP-(5-Br)T1),** 646 mg (2.196 mmol) of 5-hexyl-2-thiopheneboronic acid pinacol ester, phase-transfer catalyst (Aliquat 336, 2 drops) and 3 ml of 2M solution of K$_2$CO$_3$. After 10 minutes of stirring at room temperature, 278 mg (0.241 mmol) of Pd(PPh$_3$)$_4$ were added. The resulting mixture was stirred at reflux for 6 h. After cooling to room temperature, the mixture was poured into 50 ml of water. Phases were separated and the water phase was additionally extracted with CHCl$_3$. The collected organic

phases were washed with saturated solution of NaCl and dried over $MgSO_4$. The organic solvent was removed and the crude product was purified by column chromatography (silica gel; $CHCl_3$:CCl_4, 2:3 (v/v)) yielding 400 mg (62% yield) of black powder.

^{1}HNMR (300 MHz, $CDCl_3$), δ [ppm]: 8.92 (s, 2H), 7.23 (d, J=4.50 Hz, 2H), 7.14-7.11 (m, 2H), 6.74 (d, J=3.50 Hz, 2H), 4.08 (t, J=7.50 Hz, 4H), 2.82 (t, J=6.50 Hz, 4H), 1.75-1.66 (m, 8H), 1.46-1.20 (m, 32H), 0.91-0.82 (m, 12H). ^{13}CNMR (125 MHz, $CDCl_3$), δ [ppm]: 161.31, 147.88, 143.51, 139.06, 136.62, 133.61, 127.50, 125.38, 124.23, 123.38, 107.99, 42.29, 31.95, 31.83, 31.57, 30.33, 30.04, 29.72, 29.67, 29.39, 29.23, 26.92, 22.72, 14.13, 14.09. MS (TOF - ES^+, m/z): calculated for $C_{50}H_{68}N_2O_2S_4$ $(M+Na)^+$: 879.406, found 879.404.

3,6-bis(5'-hexyl-2,2'-bithiophen-5-yl)-2,5-di(2-ethylhexyl)-pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione (T2-A) was synthesized according to the method published in [9].

A 50 ml flask was charged under argon with 15 ml of toluene, 201 mg (0.294 mmol) of **T1-Br**, 257 mg (0.873 mmol) of 5-hexyl-2-thiopheneboronic acid pinacol ester, phase-transfer catalyst (Aliquat 336, 2 drops) and 1.5 ml of 2M solution of K_2CO_3. After purging the reaction mixture with argon for 10 minutes at room temperature, 100 mg (0.087 mmol) of $Pd(PPh_3)_4$ was added. The mixture was stirred at reflux for 6 h. After cooling to room temperature, the mixture was poured into 100 ml of water. The phases were separated and the water phase was extracted several times with $CHCl_3$. The collected organic phases were washed with saturated solution of NaCl and dried over $MgSO_4$. The organic solvent was evaporated and the crude product was dissolved in CH_2Cl_2 and precipitated with MeOH. The obtained precipitate was purified by column chromatography (silica gel, n-hexane:$CHCl_3$, 1:1 (v/v)) yielding 205 mg (80% yield) of black powder.

^{1}HNMR (400MHz, $CDCl_3$), δ [ppm]: 8.92 (s, 2H), 7.22 (d, J=4.20 Hz, 2H), 7.13 (s, 2H), 6.74 (s, 2H), 4.09-3.98 (m, 4H), 2.82 (s, 4H), 1.97-1.86 (m, 2H), 1.70-1.65 (m, 4H), 1.44-1.24 (m, 28H), 0.94-0.85 (m, 18H). ^{13}CNMR (100 MHz, $CDCl_3$), δ [ppm]: 161.62, 147.73, 143.31, 139.39, 136.70, 133.60, 127.47, 125.31, 124.91, 123.98, 108.12, 45.97, 39.25, 31.55, 31.53, 30.37, 30.31, 28.75, 28.56, 23.70, 23.13, 22.57, 14.09, 10.60. Elemental analysis calculated for $C_{50}H_{68}N_2O_2S_4$: %C: 70.00 (calc. 70.04), %H: 7.85 (calc. 8.00), %N: 3.29 (calc. 3.27), %S: 15.09 (calc. 14.96)

The synthetic procedure of **3,6-bis(3'-hexyl-2,2'-bithiophen-5-yl)-2,5-dioctyl-pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione (T2-D)** was based on these published for its alkyl analogues, i.e. [9].

A round bottom flask was charged under argon with 30 ml of toluene, 300 mg (0.439 mmol) of **(Oc-DPP-(5-Br)T1),** 387 mg (1.317 mmol) of 3-hexyl-2-thiopheneboronic acid pinacol ester, phase-transfer catalyst (Aliquat 336, 2 drops) and 3 ml of 2M solution of K_2CO_3. After 10 minutes of stirring at room temperature, 169 mg (0.146 mmol) of $Pd(PPh_3)_4$ was added. The mixture was stirred at reflux for 6 h. After cooling to room temperature, the mixture was poured into 50 ml of water and phases were separated. The water phase was additionally extracted with $CHCl_3$, the collected organic phases were washed with saturated solution of NaCl and dried over $MgSO_4$. The organic solvent was removed and the crude product was purified by column chromatography (silica gel, n-hexane:CH_2Cl_2, 1:2 (v/v)) yielding 140 mg (36% yield) of black powder.

^{1}HNMR (500 MHz, $CDCl_3$), δ [ppm]: 9.02 (d, J=4.00 Hz, 2H), 7.28 (d, J=4.00 Hz, 2H), 7.27 (d, J=4.00 Hz, 2H), 6.98 (d, J=5.00 Hz, 2H), 4.10 (t, J=8.00 Hz, 4H), 2.83 (t, J=8.00 Hz, 4H), 1.81-1.75 (m, 4H), 1.67 (quint., J=7.00 Hz, 4H), 1.47-1.24 (m, 32H), 0.93-0.85 (m, 12H). ^{13}CNMR (125 MHz, $CDCl_3$), δ [ppm]: 161.31, 142.24, 141.30, 139.30, 136.30, 130.61, 129.71, 128.83, 126.89, 125.29, 107.96, 42.38, 31.81, 31.72, 30.57, 30.14, 29.70, 29.32,

29.30, 29.26, 26.98, 22.65 (4C), 14.10 (4C). MS (TOF - ES$^+$, m/z): calculated for C$_{50}$H$_{68}$N$_2$O$_2$S$_4$ (M+Na)$^+$: 879.406, found 879.404.

3,6-bis(3'-hexyl-2,2'-bithiophen-5-yl)-2,5-di(2-ethylhexyl)-pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione (T2-C) was syntesized according to the procedure published in [9].

A 100 ml flask was charged under argon with 20 ml of toluene, 207 mg (0.304 mmol) of **(T1-Br)**, 257 mg (0.873 mmol) of 3-hexyl-2-thiopheneboronic acid pinacol ester, phase-transfer catalyst (Aliquat 336, 2 drops) and 1.5 ml of 2M solution of K$_2$CO$_3$. After purging the reaction mixture with argon for 10 minutes at room temperature, 81 mg (0.070 mmol) of Pd(PPh$_3$)$_4$ was added. The mixture was stirred at 95 ^{o}C for 9 h. After cooling to room temperature, the mixture was poured into 50 ml of water. The phases were separated and the water phase was extracted several times with CHCl$_3$. The collected organic phases were washed with saturated solution of NaCl and dried over MgSO$_4$. The organic solvent was evaporated and the crude product was purified by column chromatography (silica gel, CH$_2$Cl$_2$). Then, the product was dissolved in CHCl$_3$, precipitated with MeOH and vacuum dried, yielding 180 mg (68% yield) of brown powder

^{1}HNMR (500 MHz, CDCl$_3$), δ [ppm]: 9.02 (d, J=5.00 Hz, 2H), 7.28 (d, J=4.00 Hz, 2H), 7.25 (d, J=2.50 Hz, 2H), 6.98 (d, J=5.50 Hz, 2H), 4.06 (t, J=7.50 Hz, 4H), 2.83 (t, J=7.50 Hz, 4H), 1.98-1.93 (m, 2H), 1.67 (quin., J=5.50 Hz, 4H), 1.45-1.25 (m, 28H), 0.93-0.85 (m, 18H). ^{13}CNMR (125 MHz, CDCl$_3$), δ [ppm]: 161.69, 142.10, 141.20, 139.70, 136.44, 130.56, 129.75, 128.87, 126.69, 125.22, 108.13, 46.07, 39.29, 31.71, 30.55, 30.27, 30.25, 29.66, 29.31, 28.43, 23.58, 23.15, 22.65, 14.09, 14.07, 10.53. Elemental analysis calculated for C$_{50}$H$_{68}$N$_2$O$_2$S$_4$: %C: 69.97 (calc. 70.04), %H: 7.91 (calc. 8.00), %N: 3.33 (calc. 3.27), %S: 15.07 (calc. 14.96).

The synthetic procedure of **3,6-bis(5''-hexyl-2,2':5':2''-terthiophen-5-yl)-2,5-dioctyl-pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione (T3-B)** was based on these published for its different alkyl analogues, i.e. [10].

A round bottom flask was charged under argon with 50 ml of toluene, 300 mg (0.439 mmol) of **(Oc-DPP-(5-Br)T1),** 496 mg (1.317 mmol) of 5'-hexyl-2,2'-bithiophene-5-boronic acid pinacol ester, phase-transfer catalyst (Aliquat 336, 2 drops) and 5 ml of 2M solution of K$_2$CO$_3$. After 10 minutes of stirring at room temperature, 169 mg (0.146 mmol) of Pd(PPh$_3$)$_4$ was added. The mixture was stirred at reflux for 7 h. After cooling to room temperature, the mixture was poured into 50 ml of water. Phases were separated and the water phase was additionally extracted with CHCl$_3$. The collected organic phases were washed with saturated solution of NaCl and dried over MgSO$_4$. The organic solvent was removed and the crude product was purified by crystallization from CHCl$_3$ yielding 140 mg (31% yield) of dark green powder.

^{1}HNMR (500 MHz, CDCl$_3$), δ [ppm]: 8.93 (d, J=4.00 Hz, 2H), 7.27 (d, J=4.50 Hz, 2H), 7.20 (d, J=4.00 Hz, 2H), 7.04-7.02 (m, 4H), 6.70 (d, J=3.50 Hz, 2H), 4.09 (t, J=8.00 Hz, 4H), 2.80 (t, J=7.50 Hz, 4H), 1.78 (quint., J=7.50 Hz, 4H), 1.69 (quint., J=7.00 Hz, 4H), 1.49-1.25 (m, 32H), 0.91-0.86 (m, 12H). ^{13}CNMR (125 MHz, CDCl$_3$), δ [ppm]: 161.21, 146.46, 142.68, 138.98, 138.83, 136.62, 134.00, 127.88, 125.89, 125.03, 124.60, 124.00, 123.80, 123.75, 108.18, 42.29, 31.82, 31.56 (4C), 30.23, 30.04, 29.71, 29.23, 28.76, 26.92, 22.65, 22.58, 14.12, 14.09. MS (TOF - ES$^+$, m/z): calculated for C$_{58}$H$_{72}$N$_2$O$_2$S$_6$ (M+Na)$^+$: 1043.381, found 1043.380.

Elemental analysis: %C: 68.14 (calc. 68.19), %H: 6.98 (calc. 7.10), %S: 19.23 (calc. 18.83), %N: 2.76 (calc. 2.74).

3,6-bis(5''-hexyl-2,2':5':2''-terthiophen-5-yl)-2,5-di(2-ethylhexyl)-pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione (T3-A) was synthesized according to the method presented in [10].

A 100 ml flask was charged under argon with 20 ml of toluene, 182 mg (0.266 mmol) of **T1-Br**, 300 mg (0.797 mmol) of 5′-hexyl-2,2′-bithiophene-5-boronic acid pinacol ester, phase-transfer catalyst (Aliquat 336, 2 drops) and 1.5 ml of 2M solution of K_2CO_3. After purging the reaction mixture with argon for 10 minutes at room temperature, 100 mg (0.087 mmol) of $Pd(PPh_3)_4$ was added. The mixture was stirred at 110°C for 5 h. After cooling to room temperature, the mixture was poured into 50 ml of water. The phases were separated and the water phase was extracted several times with $CHCl_3$. The collected organic phases were washed with saturated solution of NaCl and dried over $MgSO_4$. The organic solvent was evaporated and the crude product was dissolved in $CHCl_3$ and precipitated by adding MeOH. Then, the obtained precipitate was further purified by column chromatography (silica gel, n-hexane:CH_2Cl_2, 1:1 (v/v)) yielding 178 mg (65% yield) of dark brown powder.

^{1}HNMR (400 MHz, $CDCl_3$), δ [ppm]: 8.95 (d, J=4.00 Hz, 2H), 7.25 (d, J=4.00 Hz, 2H), 7.18 (d, J=4.00 Hz, 2H), 7.04 -7.01 (m, 4H), 6.70 (d, J=4.00 Hz, 2H), 4.09-3.98 (m, 4H), 2.80 (t, J=8.00 Hz, 4H), 1.93 (quint., J=8.00 Hz, 2H), 1.69 (quint., J=8.00 Hz, 4H), 1.46-1.24 (m, 28H), 0.96-0.86 (m, 18H). ^{13}CNMR (100 MHz, $CDCl_3$), δ [ppm]: 161.53, 146.37, 142.50, 139.16, 138.84, 136.77, 134.00, 133.98, 127.86, 125.74, 124.99, 124.37, 123.92, 123.77, 108.29, 45.96, 39.28, 31.54, 30.37, 30.23, 28.77, 28.57, 28.76, 23.69, 23.15, 22.58, 14.14, 14.10, 10.60. Elemental analysis calculated for $C_{58}H_{72}N_2O_2S_6$: %C: 68.03 (calc. 68.19), %H: 6.92 (calc. 7.10), %N: 2.78 (calc. 2.74), %S: 18.99 (calc. 18.84).

2. Cyclic voltammetry of n-octyl substituted derivatives of T1, T2 and T3 compounds

a)   b)

c)   d)
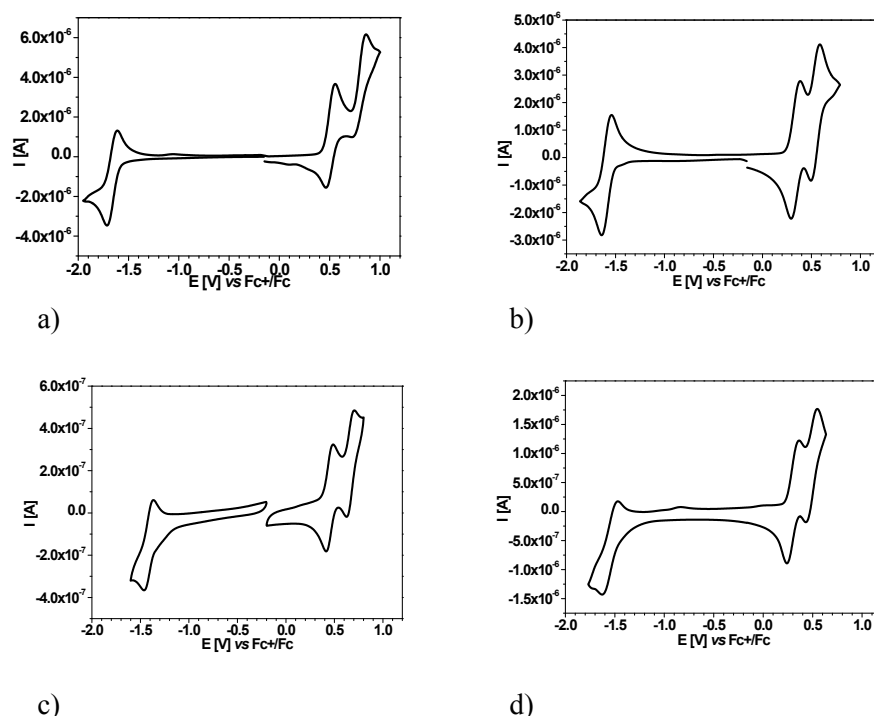
Fig. S1 Cyclic voltammograms of: a) **T1-B**; b) **T2-D**; c) **T2-B**; d) **T3-B**. Electrolyte Bu_4NBF_4/CH_2Cl_2; E *vs* Fc/Fc[+], scan rate 50 mVs[-1].

3. Experimental absorption and emission spectra

Solution (solid line) and solid state (dotted line) absorption (a) and emission (b) spectra of **T1-B**.
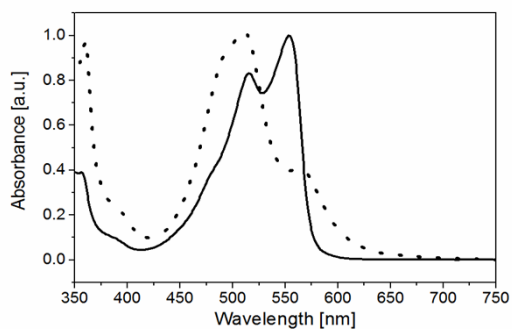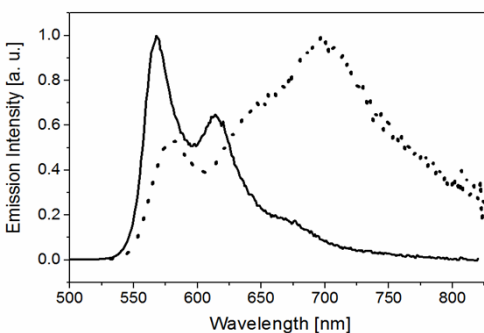
Solution (solid line) and solid state (dotted line) absorption (a) and emission (b) spectra of **T1-A**.
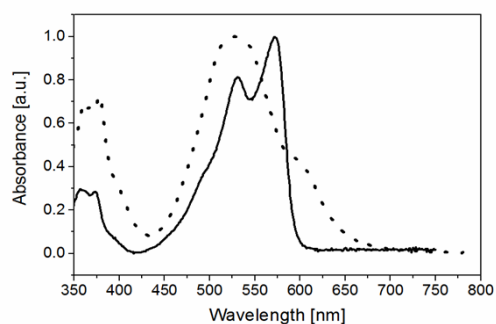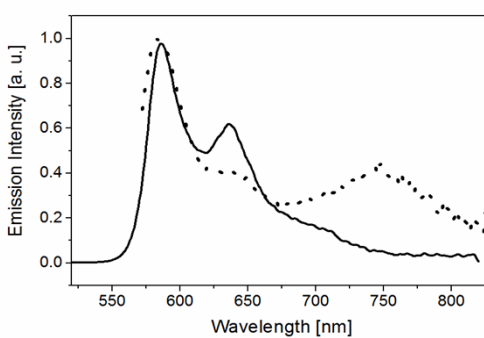
Solution (solid line) and solid state (dotted line) absorption (a) and emission (b) spectra of **T1-Br**.
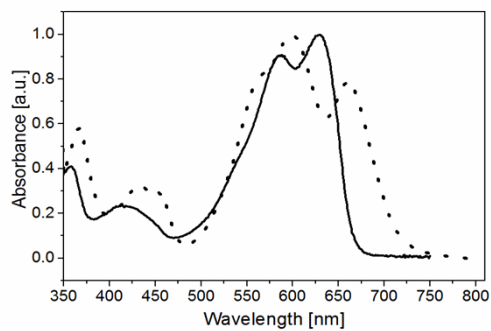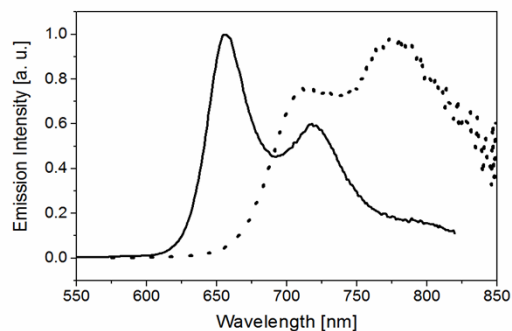
Solution (solid line) and solid state (dotted line) absorption (a) and emission (b) spectra of **T2-A**.
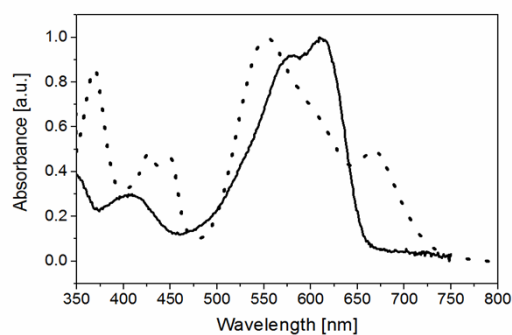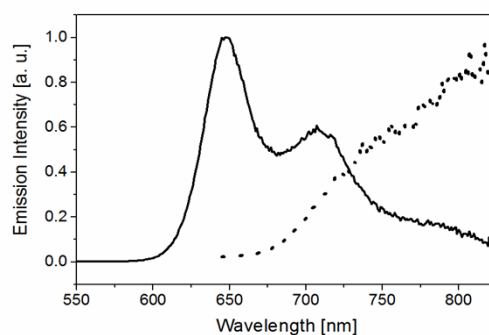
Solution (solid line) and solid state (dotted line) absorption (a) and emission (b) spectra of **T2-D**.
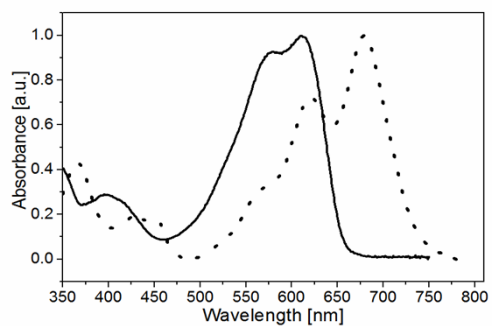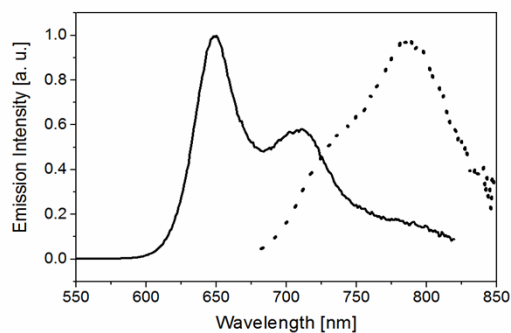
Solution (solid line) and solid state (dottted line) absorption (a) and emission (b) spectra of **T2-C**.

a   b
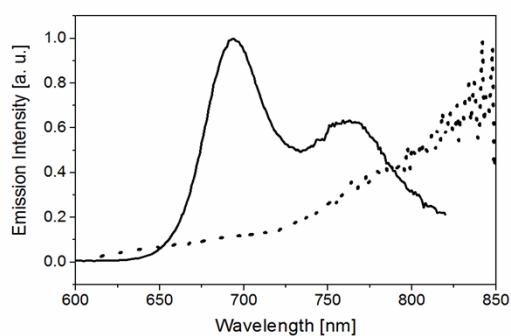
Solution (solid line) and solid state (dotted line) absorption (a) and emission (b) spectra of **T3-B**.
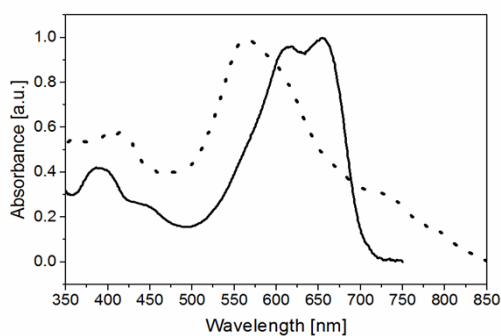
a   b
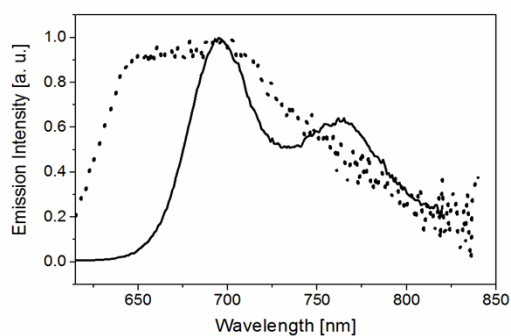
Solution (solid line) and solid state (dotted line) absorption (a) and emission (b) spectra of **T3-A**.

Fig. S2 Absorption and emission spectra of the studied compounds.

4. Calculated molecular geometries

Table S1. *Torsion angles S-C-C-S between neighbouring thiophenes, N-C-C-S between the central unit and adjacent thiophenes, and C-N-C-C between the central unit and aliphatic substituents, method: B3LYP/6-31G(d,p) in vacuum.*

Torsion angle	T1-B	T2-B	T2-D	T3-B	T1-A	T2-A	T2-C	T3-A
S-C-C-S	--	--	--	-166.6	--	--	--	167.0
S-C-C-S	--	-176.6	**145.7**	173.5	--	-172.5	**145.9**	-172.3
N-C-C-S	2.1	0.3	-1.6	0.8	-8.0	-7.2	-8.9	-7.1
C-N-C-C	*91.3*	*91.5*	*91.7*	*91.6*	*102.3*	*102.0*	*102.2*	*102.1*
C-N-C-C	*91.3*	*91.5*	*91.7*	*91.6*	*102.3*	*102.0*	*102.2*	*102.1*
N-C-C-S	2.1	0.3	-1.6	0.8	-8.0	-7.2	-8.9	-7.1
S-C-C-S	--	-176.6	**145.7**	173.5	--	-172.5	**145.9**	-172.3
S-C-C-S	--	--	--	-166.6	--	--	--	167.0

Table S2. *Bond lengths calculated for T1-A, T1-B, T2-A, T2-B, T2-C, T2-D, T3-A and T3-B by B3LYP/6-31G(d,p) method in vacuum; abbreviations used in table are explained in scheme below.*

	i	j	T1-B	T1-A	T2-B	T2-A	T2-D	T2-C	T3-B	T3-A
α	5	1	1.394	1.396	1.396	1.398	1.396	1.398	1.396	1.398
	5	4	1.396	1.395	1.400	1.399	1.399	1.397	1.400	1.400
	4	3	1.422	1.421	1.419	1.419	1.420	1.420	1.418	1.418
	3	2	1.445	1.445	1.445	1.445	1.445	1.445	1.445	1.445
	2	2a	1.230	1.231	1.231	1.231	1.231	1.231	1.231	1.231
	2	1	1.435	1.435	1.433	1.433	1.434	1.434	1.432	1.433
α–β			1.443	1.444	1.437	1.437	1.439	1.439	1.436	1.436
β	5	1	1.764	1.763	1.765	1.765	1.762	1.762	1.765	1.765
	5	4	1.389	1.389	1.391	1.391	1.391	1.391	1.392	1.392
	4	3	1.416	1.416	1.406	1.406	1.407	1.407	1.405	1.405
	3	2	1.371	1.371	1.385	1.385	1.385	1.385	1.386	1.387
	2	1	1.727	1.727	1.751	1.750	1.751	1.751	1.752	1.751
β–γ			-	-	1.443	1.443	1.452	1.452	1.439	1.439
γ	5	1	-	-	1.759	1.759	1.762	1.762	1.759	1.759
	5	4	-	-	1.380	1.380	1.387	1.387	1.383	1.383
	4	3	-	-	1.420	1.420	1.431	1.431	1.413	1.413
	3	2	-	-	1.372	1.372	1.365	1.365	1.382	1.382
	2	1	-	-	1.750	1.750	1.729	1.729	1.756	1.756
γ–δ			-	-	-	-	-	-	1.445	1.445
δ	5	1	-	-	-	-	-	-	1.759	1.759
	5	4	-	-	-	-	-	-	1.378	1.378
	4	3	-	-	-	-	-	-	1.421	1.421
	3	2	-	-	-	-	-	-	1.371	1.371
	2	1	-	-	-	-	-	-	1.751	1.751
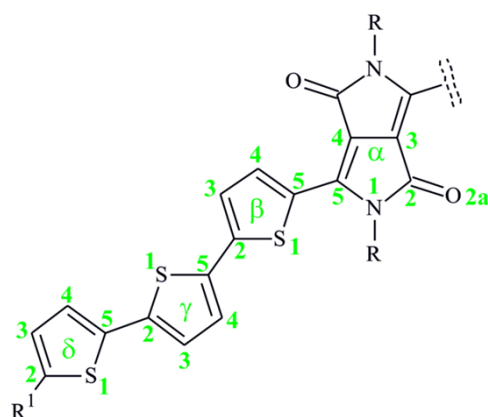
Equilibrium cartesian coordinates of all molecules

Label of each DPP derivative is followed by a list of atoms in the format:
Atomic symbol   Number   X,Y,Z coordinates in Ångströms.

a) Molecular geometries in vacuum calculated by B3LYP/6-31G(d,p) method

```
T1-B
C      1    -0.710576     0.020136    -1.312871
C      2     0.710576    -0.020136    -1.312871
C      3    -1.121635     1.405049    -1.317704
C      4     1.121635    -1.405049    -1.317704
C      5     1.213160     1.282661    -1.313531
C      6    -1.213160    -1.282661    -1.313531
N      7     0.111731     2.137575    -1.322710
N      8    -0.111731    -2.137575    -1.322710
O      9    -2.216219     1.966603    -1.322159
O     10     2.216219    -1.966603    -1.322159
C     11     2.605797     1.661403    -1.315943
C     12    -2.605797    -1.661403    -1.315943
S     13     3.229457     3.310668    -1.279419
S     14    -3.229457    -3.310668    -1.279419
C     15     4.863549     2.751814    -1.301989
C     16    -4.863549    -2.751814    -1.301989
C     17     4.935063     1.383532    -1.334302
C     18    -4.935063    -1.383532    -1.334302
C     19     3.663112     0.761656    -1.341131
C     20    -3.663112    -0.761656    -1.341131
H     21     5.672917     3.468749    -1.290767
H     22    -5.672917    -3.468749    -1.290767
H     23     5.869990     0.835993    -1.351801
H     24    -5.869990    -0.835993    -1.351801
H     25     3.501748    -0.311609    -1.361418
H     26    -3.501748     0.311609    -1.361418
C     27     0.053567     3.596923    -1.301139
C     28    -0.053567    -3.596923    -1.301139
C     29     0.077820     4.192231     0.113431
C     30    -0.077820    -4.192231     0.113431
C     31    -0.004940     5.722992     0.096331
C     32     0.004940    -5.722992     0.096331
C     33    -0.016795     6.344433     1.498433
C     34     0.016795    -6.344433     1.498433
C     35    -0.098833     7.875717     1.486886
C     36     0.098833    -7.875717     1.486886
C     37    -0.111731     8.499854     2.887482
C     38     0.111731    -8.499854     2.887482
C     39    -0.193877    10.031233     2.876631
C     40     0.193877   -10.031233     2.876631
C     41    -0.206425    10.646866     4.278961
C     42     0.206425   -10.646866     4.278961
H     43    -0.892629     3.854488    -1.784307
```

```
H    44     0.892629    -3.854488    -1.784307
H    45     0.857525     4.001014    -1.921512
H    46    -0.857525    -4.001014    -1.921512
H    47    -0.769927     3.777630     0.671635
H    48     0.769927    -3.777630     0.671635
H    49     0.989036     3.875188     0.635124
H    50    -0.989036    -3.875188     0.635124
H    51    -0.910036     6.032121    -0.445189
H    52     0.910036    -6.032121    -0.445189
H    53     0.843924     6.128810    -0.472623
H    54    -0.843924    -6.128810    -0.472623
H    55    -0.865909     5.938966     2.066199
H    56     0.865909    -5.938966     2.066199
H    57     0.886987     6.032732     2.040824
H    58    -0.886987    -6.032732     2.040824
H    59    -1.002487     8.186161     0.943194
H    60     1.002487    -8.186161     0.943194
H    61     0.750184     8.280342     0.917408
H    62    -0.750184    -8.280342     0.917408
H    63    -0.960781     8.096079     3.457475
H    64     0.960781    -8.096079     3.457475
H    65     0.791722     8.189880     3.432157
H    66    -0.791722    -8.189880     3.432157
H    67    -1.096827    10.340683     2.332868
H    68     1.096827   -10.340683     2.332868
H    69     0.654674    10.434598     2.307300
H    70    -0.654674   -10.434598     2.307300
H    71    -1.063789    10.289808     4.860833
H    72     1.063789   -10.289808     4.860833
H    73     0.700675    10.384335     4.835244
H    74    -0.700675   -10.384335     4.835244
H    75    -0.265582    11.739330     4.237027
H    76     0.265582   -11.739330     4.237027

T1-A
C     1    -0.707269     0.069844    -0.856743
C     2     0.707269    -0.069844    -0.856743
C     3    -1.020842     1.479901    -0.891371
C     4     1.020842    -1.479901    -0.891371
C     5     1.298180     1.193164    -0.910857
C     6    -1.298180    -1.193164    -0.910857
N     7     0.259952     2.126847    -0.903113
N     8    -0.259952    -2.126847    -0.903113
O     9    -2.080016     2.106393    -0.897239
O    10     2.080016    -2.106393    -0.897239
C    11     2.711070     1.470543    -1.014764
C    12    -2.711070    -1.470543    -1.014764
S    13     3.429335     3.044507    -1.353578
S    14    -3.429335    -3.044507    -1.353578
C    15     5.022346     2.377325    -1.359041
C    16    -5.022346    -2.377325    -1.359041
```

```
C    17     5.012592     1.028205    -1.117572
C    18    -5.012592    -1.028205    -1.117572
C    19     3.709213     0.509384    -0.926355
C    20    -3.709213    -0.509384    -0.926355
H    21     5.870799     3.023276    -1.538257
H    22    -5.870799    -3.023276    -1.538257
H    23     5.910580     0.423055    -1.078448
H    24    -5.910580    -0.423055    -1.078448
H    25     3.483070    -0.536797    -0.749434
H    26    -3.483070     0.536797    -0.749434
C    27     0.323611     3.584489    -0.809314
C    28    -0.323611    -3.584489    -0.809314
C    29     0.707269     4.135966     0.584353
C    30    -0.707269    -4.135966     0.584353
C    31     0.924412     5.658720     0.464007
C    32    -0.924412    -5.658720     0.464007
C    33     1.431488     6.342090     1.740501
C    34    -1.431488    -6.342090     1.740501
C    35     1.753288     7.828661     1.539144
C    36    -1.753288    -7.828661     1.539144
C    37     2.254398     8.515955     2.812748
C    38    -2.254398    -8.515955     2.812748
C    39    -0.288199     3.727436     1.694272
C    40     0.288199    -3.727436     1.694272
C    41    -1.690404     4.344021     1.612881
C    42     1.690404    -4.344021     1.612881
H    43    -0.675852     3.925460    -1.089683
H    44     0.675852    -3.925460    -1.089683
H    45     1.012764     3.964775    -1.569023
H    46    -1.012764    -3.964775    -1.569023
H    47     2.476164     9.573529     2.636666
H    48    -2.476164    -9.573529     2.636666
H    49     1.675514     3.693398     0.855230
H    50    -1.675514    -3.693398     0.855230
H    51    -0.007054     6.141620     0.138254
H    52     0.007054    -6.141620     0.138254
H    53     1.651555     5.840853    -0.339861
H    54    -1.651555    -5.840853    -0.339861
H    55     0.686805     6.245105     2.540928
H    56    -0.686805    -6.245105     2.540928
H    57     2.331988     5.822154     2.097858
H    58    -2.331988    -5.822154     2.097858
H    59     0.856253     8.346194     1.172736
H    60    -0.856253    -8.346194     1.172736
H    61     2.506683     7.931919     0.746338
H    62    -2.506683    -7.931919     0.746338
H    63     1.507207     8.461912     3.612638
H    64    -1.507207    -8.461912     3.612638
H    65     3.169711     8.041902     3.185083
H    66    -3.169711    -8.041902     3.185083
H    67     0.162127     3.980799     2.661457
```

```
H    68    -0.162127    -3.980799     2.661457
H    69    -0.377694     2.634338     1.692871
H    70     0.377694    -2.634338     1.692871
H    71    -1.661416     5.437916     1.658894
H    72     1.661416    -5.437916     1.658894
H    73    -2.206409     4.047387     0.696153
H    74     2.206409    -4.047387     0.696153
H    75    -2.300099     4.000736     2.455215
H    76     2.300099    -4.000736     2.455215

T2-B
C     1    -0.542942    -0.456870    -0.317587
C     2     0.542942     0.456870    -0.317587
C     3    -1.771913     0.302509    -0.323346
C     4     1.771913    -0.302509    -0.323346
C     5     0.051185     1.767408    -0.323934
C     6    -0.051185    -1.767408    -0.323934
N     7    -1.341234     1.669153    -0.333601
N     8     1.341234    -1.669153    -0.333601
O     9    -2.962654    -0.009653    -0.319793
O    10     2.962654     0.009653    -0.319793
C    11     0.835562     2.970861    -0.335126
C    12    -0.835562    -2.970861    -0.335126
S    13     0.202627     4.618641    -0.356862
S    14    -0.202627    -4.618641    -0.356862
C    15     1.811093     5.310092    -0.357723
C    16    -1.811093    -5.310092    -0.357723
C    17     2.763093     4.304336    -0.345640
C    18    -2.763093    -4.304336    -0.345640
C    19     2.226591     3.004753    -0.332902
C    20    -2.226591    -3.004753    -0.332902
C    21     2.001310     6.740332    -0.372453
C    22    -2.001310    -6.740332    -0.372453
H    23     3.828256     4.505927    -0.341175
H    24    -3.828256    -4.505927    -0.341175
H    25     2.820040     2.095719    -0.321318
H    26    -2.820040    -2.095719    -0.321318
C    27    -2.355840     2.718191    -0.284831
C    28     2.355840    -2.718191    -0.284831
C    29    -2.695332     3.176662     1.140179
C    30     2.695332    -3.176662     1.140179
C    31    -3.776417     4.263481     1.156885
C    32     3.776417    -4.263481     1.156885
C    33    -4.157741     4.714560     2.572293
C    34     4.157741    -4.714560     2.572293
C    35    -5.237507     5.803196     2.597827
C    36     5.237507    -5.803196     2.597827
C    37    -5.620512     6.253012     4.012894
C    38     5.620512    -6.253012     4.012894
C    39    -6.699862     7.342130     4.040855
C    40     6.699862    -7.342130     4.040855
```

```
C     41    -7.076494     7.784862     5.457849
C     42     7.076494    -7.784862     5.457849
H     43    -3.245033     2.279234    -0.744913
H     44     3.245033    -2.279234    -0.744913
H     45    -2.043763     3.556306    -0.913284
H     46     2.043763    -3.556306    -0.913284
H     47    -3.035750     2.301864     1.706864
H     48     3.035750    -2.301864     1.706864
H     49    -1.789982     3.546149     1.636915
H     50     1.789982    -3.546149     1.636915
H     51    -4.672897     3.893310     0.639875
H     52     4.672897    -3.893310     0.639875
H     53    -3.429682     5.133217     0.580287
H     54     3.429682    -5.133217     0.580287
H     55    -4.505151     3.844631     3.146980
H     56     4.505151    -3.844631     3.146980
H     57    -3.259994     5.080735     3.090068
H     58     3.259994    -5.080735     3.090068
H     59    -6.134443     5.436683     2.078462
H     60     6.134443    -5.436683     2.078462
H     61    -4.889722     6.673206     2.022410
H     62     4.889722    -6.673206     2.022410
H     63    -5.969141     5.383550     4.588459
H     64     5.969141    -5.383550     4.588459
H     65    -4.723746     6.619016     4.533293
H     66     4.723746    -6.619016     4.533293
H     67    -7.595938     6.976200     3.521334
H     68     7.595938    -6.976200     3.521334
H     69    -6.351365     8.211225     3.466254
H     70     6.351365    -8.211225     3.466254
H     71    -7.461987     6.944412     6.046211
H     72     7.461987    -6.944412     6.046211
H     73    -6.208089     8.188367     5.991015
H     74     6.208089    -8.188367     5.991015
H     75    -7.847902     8.561726     5.443885
H     76     7.847902    -8.561726     5.443885
S     77     3.614797     7.435955    -0.461913
C     78     2.988231     9.069572    -0.427998
C     79     1.618103     9.051855    -0.355617
C     80     1.058855     7.746697    -0.323605
H     81    -0.006318     7.553549    -0.260371
H     82     1.024945     9.959337    -0.321165
C     83     3.903618    10.257886    -0.498644
C     84     4.588393    10.452636    -1.867168
C     85     5.486803    11.693977    -1.910454
C     86     6.176974    11.898236    -3.264537
C     87     7.076494    13.139517    -3.312558
C     88     7.762163    13.336553    -4.667756
H     89     3.309183    11.148317    -0.260429
H     90     4.674608    10.186495     0.280316
H     91     3.816724    10.522495    -2.644302
```

```
H    92     5.181928      9.560432     -2.105378
H    93     4.888685     12.584513     -1.669646
H    94     6.248988     11.619032     -1.121671
H    95     5.414921     11.972383     -4.053362
H    96     6.775179     11.007950     -3.505349
H    97     6.478276     14.028899     -3.071920
H    98     7.837865     13.064772     -2.524245
H    99     7.026056     13.449673     -5.471736
H   100     8.395609     12.478565     -4.919933
H   101     8.395987     14.229174     -4.669903
S   102    -3.614797     -7.435955     -0.461913
C   103    -2.988231     -9.069572     -0.427998
C   104    -1.618103     -9.051855     -0.355617
C   105    -1.058855     -7.746697     -0.323605
H   106     0.006318     -7.553549     -0.260371
H   107    -1.024945     -9.959337     -0.321165
C   108    -3.903618    -10.257886     -0.498644
C   109    -4.588393    -10.452636     -1.867168
C   110    -5.486803    -11.693977     -1.910454
C   111    -6.176974    -11.898236     -3.264537
C   112    -7.076494    -13.139517     -3.312558
C   113    -7.762163    -13.336553     -4.667756
H   114    -4.674608    -10.186495      0.280316
H   115    -3.309183    -11.148317     -0.260429
H   116    -5.181928     -9.560432     -2.105378
H   117    -3.816724    -10.522495     -2.644302
H   118    -6.248988    -11.619032     -1.121671
H   119    -4.888685    -12.584513     -1.669646
H   120    -6.775179    -11.007950     -3.505349
H   121    -5.414921    -11.972383     -4.053362
H   122    -7.837865    -13.064772     -2.524245
H   123    -6.478276    -14.028899     -3.071920
H   124    -8.395609    -12.478565     -4.919933
H   125    -7.026056    -13.449673     -5.471736
H   126    -8.395987    -14.229174     -4.669903

T2-A
C     1    -0.355919     -0.613760     -0.437502
C     2     0.355919      0.613760     -0.437502
C     3    -1.769301     -0.316442     -0.472024
C     4     1.769301      0.316442     -0.472024
C     5    -0.550460      1.678096     -0.490817
C     6     0.550460     -1.678096     -0.490817
N     7    -1.830108      1.115546     -0.482831
N     8     1.830108     -1.115546     -0.482831
O     9    -2.777580     -1.023469     -0.478869
O    10     2.777580      1.023469     -0.478869
C    11    -0.219279      3.072448     -0.595446
C    12     0.219279     -3.072448     -0.595446
S    13    -1.358459      4.381023     -0.917877
S    14     1.358459     -4.381023     -0.917877
```

```
C      15    -0.084320     5.581317    -0.922864
C      16     0.084320    -5.581317    -0.922864
C      17     1.141845     4.978081    -0.697622
C      18    -1.141845    -4.978081    -0.697622
C      19     1.072083     3.585072    -0.519721
C      20    -1.072083    -3.585072    -0.519721
C      21    -0.383619     6.975708    -1.142800
C      22     0.383619    -6.975708    -1.142800
H      23     2.070161     5.536157    -0.653882
H      24    -2.070161    -5.536157    -0.653882
H      25     1.931833     2.944540    -0.352676
H      26    -1.931833    -2.944540    -0.352676
C      27    -3.130883     1.774943    -0.387542
C      28     3.130883    -1.774943    -0.387542
C      29    -3.476732     2.345336     1.008553
C      30     3.476732    -2.345336     1.008553
C      31    -4.772810     3.173782     0.890053
C      32     4.772810    -3.173782     0.890053
C      33    -5.188026     3.911801     2.169245
C      34     5.188026    -3.911801     2.169245
C      35    -6.407207     4.821577     1.969552
C      36     6.407207    -4.821577     1.969552
C      37    -6.829120     5.555238     3.245996
C      38     6.829120    -5.555238     3.245996
C      39    -3.519114     1.264706     2.113231
C      40     3.519114    -1.264706     2.113231
C      41    -4.660230     0.243554     2.024048
C      42     4.660230    -0.243554     2.024048
H      43    -3.854449     1.007672    -0.673366
H      44     3.854449    -1.007672    -0.673366
H      45    -3.191261     2.564136    -1.142854
H      46     3.191261    -2.564136    -1.142854
H      47    -7.699268     6.196315     3.071004
H      48     7.699268    -6.196315     3.071004
H      49    -2.673533     3.042206     1.284131
H      50     2.673533    -3.042206     1.284131
H      51    -5.597311     2.527567     0.558938
H      52     5.597311    -2.527567     0.558938
H      53    -4.635765     3.915125     0.090069
H      54     4.635765    -3.915125     0.090069
H      55    -5.410546     3.189610     2.965182
H      56     5.410546    -3.189610     2.965182
H      57    -4.342714     4.514001     2.532124
H      58     4.342714    -4.514001     2.532124
H      59    -7.248729     4.221690     1.597034
H      60     7.248729    -4.221690     1.597034
H      61    -6.186802     5.554661     1.181499
H      62     6.186802    -5.554661     1.181499
H      63    -7.092021     4.848184     4.040967
H      64     7.092021    -4.848184     4.040967
H      65    -6.019489     6.189518     3.624598
```

```
H    66     6.019489    -6.189518     3.624598
H    67    -3.565496     1.774765     3.082904
H    68     3.565496    -1.774765     3.082904
H    69    -2.561003     0.731096     2.110901
H    70     2.561003    -0.731096     2.110901
H    71    -5.644426     0.722199     2.068399
H    72     5.644426    -0.722199     2.068399
H    73    -4.599694    -0.345281     1.105275
H    74     4.599694     0.345281     1.105275
H    75    -4.602853    -0.456825     2.863895
H    76     4.602853     0.456825     2.863895
S    77     0.905523     8.155473    -1.344501
C    78    -0.233145     9.469039    -1.544042
C    79    -1.519977     8.999733    -1.460976
C    80    -1.610190     7.600431    -1.235499
H    81    -2.550368     7.069143    -1.137227
H    82    -2.383908     9.648085    -1.559983
C    83     0.233145    10.881949    -1.747224
C    84     0.865301    11.528459    -0.497287
C    85     1.296897    12.980254    -0.733880
C    86     1.927970    13.636203     0.500241
C    87     2.360511    15.089159     0.267726
C    88     2.989132    15.737674     1.504566
H    89     0.952650    10.926118    -2.575776
H    90    -0.634008    11.474747    -2.062776
H    91     1.731928    10.933504    -0.181036
H    92     0.145102    11.482746     0.329481
H    93     2.010508    13.015968    -1.569444
H    94     0.426529    13.570872    -1.053902
H    95     2.798385    13.046009     0.820415
H    96     1.214598    13.599934     1.335866
H    97     3.073744    15.124680    -0.566975
H    98     1.490464    15.678366    -0.052618
H    99     3.882223    15.191107     1.828064
H   100     2.287352    15.748909     2.346242
H   101     3.286750    16.772438     1.306622
S   102    -0.905523    -8.155473    -1.344501
C   103     0.233145    -9.469039    -1.544042
C   104     1.519977    -8.999733    -1.460976
C   105     1.610190    -7.600431    -1.235499
H   106     2.550368    -7.069143    -1.137227
H   107     2.383908    -9.648085    -1.559983
C   108    -0.233145   -10.881949    -1.747224
C   109    -0.865301   -11.528459    -0.497287
C   110    -1.296897   -12.980254    -0.733880
C   111    -1.927970   -13.636203     0.500241
C   112    -2.360511   -15.089159     0.267726
C   113    -2.989132   -15.737674     1.504566
H   114     0.634008   -11.474747    -2.062776
H   115    -0.952650   -10.926118    -2.575776
H   116    -0.145102   -11.482746     0.329481
```

```
H    117    -1.731928    -10.933504    -0.181036
H    118    -0.426529    -13.570872    -1.053902
H    119    -2.010508    -13.015968    -1.569444
H    120    -1.214598    -13.599934     1.335866
H    121    -2.798385    -13.046009     0.820415
H    122    -1.490464    -15.678366    -0.052618
H    123    -3.073744    -15.124680    -0.566975
H    124    -2.287352    -15.748909     2.346242
H    125    -3.882223    -15.191107     1.828064
H    126    -3.286750    -16.772438     1.306622

T2-D
C      1     0.654304     -0.275824    -0.550654
C      2    -0.654304      0.275824    -0.550654
C      3     1.602948      0.813819    -0.561309
C      4    -1.602948     -0.813819    -0.561309
C      5    -0.572561      1.671987    -0.566061
C      6     0.572561     -1.671987    -0.566061
N      7     0.785889      1.991699    -0.577709
N      8    -0.785889     -1.991699    -0.577709
O      9     2.832342      0.869003    -0.553562
O     10    -2.832342     -0.869003    -0.553562
C     11    -1.679812      2.590513    -0.581558
C     12     1.679812     -2.590513    -0.581558
S     13    -1.567162      4.347694    -0.659213
S     14     1.567162     -4.347694    -0.659213
C     15    -3.308201      4.533337    -0.686836
C     16     3.308201     -4.533337    -0.686836
C     17    -3.915612      3.290608    -0.615688
C     18     3.915612     -3.290608    -0.615688
C     19    -3.017435      2.209640    -0.559146
C     20     3.017435     -2.209640    -0.559146
C     21    -3.957068      5.831835    -0.708751
C     22     3.957068     -5.831835    -0.708751
H     23    -4.992690      3.170549    -0.627899
H     24     4.992690     -3.170549    -0.627899
H     25    -3.314695      1.166205    -0.521988
H     26     3.314695     -1.166205    -0.521988
C     27     1.443780      3.293583    -0.507690
C     28    -1.443780     -3.293583    -0.507690
C     29     1.602948      3.823265     0.924244
C     30    -1.602948     -3.823265     0.924244
C     31     2.328941      5.172867     0.965007
C     32    -2.328941     -5.172867     0.965007
C     33     2.529210      5.709640     2.387633
C     34    -2.529210     -5.709640     2.387633
C     35     3.256708      7.058786     2.435434
C     36    -3.256708     -7.058786     2.435434
C     37     3.457683      7.597246     3.857076
C     38    -3.457683     -7.597246     3.857076
C     39     4.185456      8.946271     3.906089
```

```
C   40   -4.185456   -8.946271    3.906089
C   41    4.380933    9.477125    5.329357
C   42   -4.380933   -9.477125    5.329357
H   43    0.912030    4.006538   -1.142958
H   44   -0.912030   -4.006538   -1.142958
H   45    2.432052    3.138325   -0.948224
H   46   -2.432052   -3.138325   -0.948224
H   47    0.618046    3.916823    1.397813
H   48   -0.618046   -3.916823    1.397813
H   49    2.165079    3.079604    1.501605
H   50   -2.165079   -3.079604    1.501605
H   51    1.763504    5.909840    0.376292
H   52   -1.763504   -5.909840    0.376292
H   53    3.306698    5.075075    0.472674
H   54   -3.306698   -5.075075    0.472674
H   55    1.551173    5.806117    2.879659
H   56   -1.551173   -5.806117    2.879659
H   57    3.093008    4.972002    2.975635
H   58   -3.093008   -4.972002    2.975635
H   59    2.693010    7.796224    1.845573
H   60   -2.693010   -7.796224    1.845573
H   61    4.234710    6.961126    1.942859
H   62   -4.234710   -6.961126    1.942859
H   63    2.479887    7.695438    4.350144
H   64   -2.479887   -7.695438    4.350144
H   65    4.020842    6.860714    4.447969
H   66   -4.020842   -6.860714    4.447969
H   67    3.623088    9.681949    3.314984
H   68   -3.623088   -9.681949    3.314984
H   69    5.163023    8.847548    3.414754
H   70   -5.163023   -8.847548    3.414754
H   71    3.418947    9.619707    5.834744
H   72   -3.418947   -9.619707    5.834744
H   73    4.970256    8.779318    5.935065
H   74   -4.970256   -8.779318    5.935065
H   75    4.902451   10.439808    5.330409
H   76   -4.902451  -10.439808    5.330409
S   77   -5.488210    5.994797    0.147948
C   78   -5.644225    7.646683   -0.337588
C   79   -4.582162    8.047686   -1.096115
C   80   -3.605749    7.025997   -1.321239
H   81   -6.507993    8.222538   -0.035715
H   82   -4.490451    9.046976   -1.508240
C   83   -2.376606    7.278767   -2.159885
C   84   -1.257671    8.029548   -1.408986
C   85   -0.039548    8.323484   -2.292287
C   86    1.076697    9.077998   -1.560124
C   87    2.297981    9.373292   -2.439495
C   88    3.407737   10.125268   -1.698894
H   89   -1.982205    6.335151   -2.550325
H   90   -2.671637    7.873550   -3.034308
```

```
H     91    -0.948127     7.439944    -0.536211
H     92    -1.659775     8.970395    -1.010236
H     93     0.358694     7.378374    -2.687992
H     94    -0.358496     8.906749    -3.168014
H     95     1.395475     8.494814    -0.683959
H     96     0.678032    10.023072    -1.164301
H     97     2.695892     8.428539    -2.834028
H     98     1.980593     9.956643    -3.314555
H     99     3.768455     9.551517    -0.837645
H    100     3.050410    11.091348    -1.324503
H    101     4.265109    10.318778    -2.351573
S    102     5.488210    -5.994797     0.147948
C    103     5.644225    -7.646683    -0.337588
C    104     4.582162    -8.047686    -1.096115
C    105     3.605749    -7.025997    -1.321239
H    106     6.507993    -8.222538    -0.035715
H    107     4.490451    -9.046976    -1.508240
C    108     2.376606    -7.278767    -2.159885
C    109     1.257671    -8.029548    -1.408986
C    110     0.039548    -8.323484    -2.292287
C    111    -1.076697    -9.077998    -1.560124
C    112    -2.297981    -9.373292    -2.439495
C    113    -3.407737   -10.125268    -1.698894
H    114     1.982205    -6.335151    -2.550325
H    115     2.671637    -7.873550    -3.034308
H    116     0.948127    -7.439944    -0.536211
H    117     1.659775    -8.970395    -1.010236
H    118    -0.358694    -7.378374    -2.687992
H    119     0.358496    -8.906749    -3.168014
H    120    -1.395475    -8.494814    -0.683959
H    121    -0.678032   -10.023072    -1.164301
H    122    -2.695892    -8.428539    -2.834028
H    123    -1.980593    -9.956643    -3.314555
H    124    -3.768455    -9.551517    -0.837645
H    125    -3.050410   -11.091348    -1.324503
H    126    -4.265109   -10.318778    -2.351573

T2-C
C      1    -0.620885    -0.344374     0.132166
C      2     0.620885     0.344374     0.132166
C      3    -1.681398     0.636437     0.092713
C      4     1.681398    -0.636437     0.092713
C      5     0.388877     1.721123     0.071280
C      6    -0.388877    -1.721123     0.071280
N      7    -0.997574     1.896672     0.076996
N      8     0.997574    -1.896672     0.076996
O      9    -2.909209     0.547401     0.087715
O     10     2.909209    -0.547401     0.087715
C     11     1.389277     2.750222    -0.033768
C     12    -1.389277    -2.750222    -0.033768
S     13     1.086139     4.446656    -0.400396
```

```
S    14    -1.086139    -4.446656    -0.400396
C    15     2.796060     4.822284    -0.434430
C    16    -2.796060    -4.822284    -0.434430
C    17     3.534630     3.684276    -0.154577
C    18    -3.534630    -3.684276    -0.154577
C    19     2.759274     2.530872     0.062372
C    20    -2.759274    -2.530872     0.062372
C    21     3.297867     6.166199    -0.657213
C    22    -3.297867    -6.166199    -0.657213
H    23     4.618192     3.687121    -0.132749
H    24    -4.618192    -3.687121    -0.132749
H    25     3.168903     1.543982     0.250260
H    26    -3.168903    -1.543982     0.250260
C    27    -1.773847     3.130433     0.185691
C    28     1.773847    -3.130433     0.185691
C    29    -1.756446     3.796311     1.582267
C    30     1.756446    -3.796311     1.582267
C    31    -2.459913     5.165413     1.478039
C    32     2.459913    -5.165413     1.478039
C    33    -2.420651     6.013185     2.755981
C    34     2.420651    -6.013185     2.755981
C    35    -3.019796     7.412851     2.566706
C    36     3.019796    -7.412851     2.566706
C    37    -2.990089     8.260643     3.841854
C    38     2.990089    -8.260643     3.841854
C    39    -2.316762     2.884510     2.697734
C    40     2.316762    -2.884510     2.697734
C    41    -3.818773     2.578781     2.638030
C    42     3.818773    -2.578781     2.638030
H    43    -2.792736     2.842783    -0.084610
H    44     2.792736    -2.842783    -0.084610
H    45    -1.432761     3.840086    -0.573894
H    46     1.432761    -3.840086    -0.573894
H    47    -3.422576     9.252316     3.673929
H    48     3.422576    -9.252316     3.673929
H    49    -0.706168     3.992678     1.837524
H    50     0.706168    -3.992678     1.837524
H    51    -3.504248     5.022992     1.167913
H    52     3.504248    -5.022992     1.167913
H    53    -1.983521     5.736319     0.668239
H    54     1.983521    -5.736319     0.668239
H    55    -2.960600     5.502109     3.563372
H    56     2.960600    -5.502109     3.563372
H    57    -1.380035     6.108227     3.097662
H    58     1.380035    -6.108227     3.097662
H    59    -4.056039     7.317844     2.214417
H    60     4.056039    -7.317844     2.214417
H    61    -2.475110     7.934776     1.767838
H    62     2.475110    -7.934776     1.767838
H    63    -3.557583     7.782878     4.648538
H    64     3.557583    -7.782878     4.648538
```

```
H     65    -1.964009      8.401664      4.200043
H     66     1.964009     -8.401664      4.200043
H     67    -2.080572      3.348127      3.662992
H     68     2.080572     -3.348127      3.662992
H     69    -1.758764      1.940433      2.684773
H     70     1.758764     -1.940433      2.684773
H     71    -4.425723      3.488597      2.696981
H     72     4.425723     -3.488597      2.696981
H     73    -4.082929      2.042326      1.723081
H     74     4.082929     -2.042326      1.723081
H     75    -4.105561      1.943330      3.482453
H     76     4.105561     -1.943330      3.482453
S     77     4.776802      6.636063      0.177447
C     78     4.761746      8.197329     -0.564780
C     79     3.683521      8.349533     -1.388478
C     80     2.833425      7.200427     -1.456801
H     81     5.547226      8.908526     -0.350168
H     82     3.492971      9.254079     -1.956196
C     83     1.607932      7.174767     -2.337421
C     84     0.388877      7.895546     -1.725738
C     85    -0.830294      7.897770     -2.655220
C     86    -2.048649      8.615611     -2.062113
C     87    -3.269275      8.621504     -2.990721
C     88    -4.481741      9.339358     -2.390622
H     89     1.858024      7.657713     -3.291135
H     90     1.335422      6.142447     -2.579379
H     91     0.667174      8.928810     -1.479158
H     92     0.126359      7.418299     -0.772558
H     93    -0.558200      8.371642     -3.609296
H     94    -1.102084      6.861123     -2.899813
H     95    -1.776096      9.651816     -1.815518
H     96    -2.322371      8.140509     -1.108940
H     97    -2.996397      9.096525     -3.942917
H     98    -3.541238      7.586031     -3.236432
H     99    -4.251641     10.387424     -2.167528
H    100    -4.799391      8.865792     -1.454780
H    101    -5.335193      9.325464     -3.076142
S    102    -4.776802     -6.636063      0.177447
C    103    -4.761746     -8.197329     -0.564780
C    104    -3.683521     -8.349533     -1.388478
C    105    -2.833425     -7.200427     -1.456801
H    106    -5.547226     -8.908526     -0.350168
H    107    -3.492971     -9.254079     -1.956196
C    108    -1.607932     -7.174767     -2.337421
C    109    -0.388877     -7.895546     -1.725738
C    110     0.830294     -7.897770     -2.655220
C    111     2.048649     -8.615611     -2.062113
C    112     3.269275     -8.621504     -2.990721
C    113     4.481741     -9.339358     -2.390622
H    114    -1.335422     -6.142447     -2.579379
H    115    -1.858024     -7.657713     -3.291135
```

H	116	-0.126359	-7.418299	-0.772558
H	117	-0.667174	-8.928810	-1.479158
H	118	1.102084	-6.861123	-2.899813
H	119	0.558200	-8.371642	-3.609296
H	120	2.322371	-8.140509	-1.108940
H	121	1.776096	-9.651816	-1.815518
H	122	3.541238	-7.586031	-3.236432
H	123	2.996397	-9.096525	-3.942917
H	124	4.799391	-8.865792	-1.454780
H	125	4.251641	-10.387424	-2.167528
H	126	5.335193	-9.325464	-3.076142

T3-B

C	1	0.427960	0.565530	-0.436031
C	2	-0.427960	-0.565530	-0.436031
C	3	1.795060	0.097383	-0.442334
C	4	-1.795060	-0.097383	-0.442334
C	5	0.342330	-1.735008	-0.441659
C	6	-0.342330	1.735008	-0.441659
N	7	1.678300	-1.330309	-0.451438
N	8	-1.678300	1.330309	-0.451438
O	9	2.886665	0.666216	-0.441694
O	10	-2.886665	-0.666216	-0.441694
C	11	-0.155873	-3.081429	-0.450172
C	12	0.155873	3.081429	-0.450172
S	13	0.826261	-4.548151	-0.455164
S	14	-0.826261	4.548151	-0.455164
C	15	-0.590086	-5.578477	-0.472467
C	16	0.590086	5.578477	-0.472467
C	17	-1.742040	-4.807019	-0.466252
C	18	1.742040	4.807019	-0.466252
C	19	-1.505929	-3.422337	-0.453597
C	20	1.505929	3.422337	-0.453597
C	21	-0.459981	-7.011834	-0.487719
C	22	0.459981	7.011834	-0.487719
H	23	-2.736374	-5.238766	-0.478978
H	24	2.736374	5.238766	-0.478978
H	25	-2.285378	-2.666573	-0.451110
H	26	2.285378	2.666573	-0.451110
C	27	2.900624	-2.128478	-0.412436
C	28	-2.900624	2.128478	-0.412436
C	29	3.345974	-2.501318	1.008412
C	30	-3.345974	2.501318	1.008412
C	31	4.640120	-3.323205	1.010850
C	32	-4.640120	3.323205	1.010850
C	33	5.124861	-3.684972	2.420215
C	34	-5.124861	3.684972	2.420215
C	35	6.417540	-4.509993	2.428633
C	36	-6.417540	4.509993	2.428633
C	37	6.903732	-4.873639	3.836725
C	38	-6.903732	4.873639	3.836725

```
C    39     8.195832    -5.699727     3.846142
C    40    -8.195832     5.699727     3.846142
C    41     8.674367    -6.059183     5.255922
C    42    -8.674367     6.059183     5.255922
H    43     3.666831    -1.503749    -0.878979
H    44    -3.666831     1.503749    -0.878979
H    45     2.776172    -3.014715    -1.040066
H    46    -2.776172     3.014715    -1.040066
H    47     3.490696    -1.573451     1.574408
H    48    -3.490696     1.573451     1.574408
H    49     2.549401    -3.061787     1.512675
H    50    -2.549401     3.061787     1.512675
H    51     5.428168    -2.762773     0.488433
H    52    -5.428168     2.762773     0.488433
H    53     4.488172    -4.245897     0.432322
H    54    -4.488172     4.245897     0.432322
H    55     5.278431    -2.762464     2.997383
H    56    -5.278431     2.762464     2.997383
H    57     4.334736    -4.241844     2.943346
H    58    -4.334736     4.241844     2.943346
H    59     7.207086    -3.952349     1.904938
H    60    -7.207086     3.952349     1.904938
H    61     6.263551    -5.431605     1.849090
H    62    -6.263551     5.431605     1.849090
H    63     7.058998    -3.952617     4.416729
H    64    -7.058998     3.952617     4.416729
H    65     6.114305    -5.430853     4.361359
H    66    -6.114305     5.430853     4.361359
H    67     8.984713    -5.142550     3.322683
H    68    -8.984713     5.142550     3.322683
H    69     8.040550    -6.619973     3.266528
H    70    -8.040550     6.619973     3.266528
H    71     8.872030    -5.158903     5.848845
H    72    -8.872030     5.158903     5.848845
H    73     7.920897    -6.647179     5.792325
H    74    -7.920897     6.647179     5.792325
H    75     9.597160    -6.647819     5.228574
H    76    -9.597160     6.647819     5.228574
S    77    -1.874349    -8.046436    -0.334048
C    78     0.680277    -7.784383    -0.609660
C    79     0.432838    -9.175198    -0.596662
C    80    -0.902925    -9.503316    -0.463476
H    81     1.211730    -9.921640    -0.702227
H    82     1.670077    -7.356711    -0.723230
S    83    -0.548998   -12.258924    -0.195891
C    84    -1.958214   -13.296310    -0.261058
C    85    -3.092289   -12.544942    -0.434738
C    86    -2.851485   -11.146903    -0.524729
C    87    -1.519348   -10.809015    -0.418959
H    88    -3.634376   -10.412224    -0.677154
H    89    -4.080192   -12.988187    -0.499658
```

25

```
C     90    -1.833830   -14.789187    -0.155754
C     91    -1.185281   -15.461515    -1.383264
C     92    -1.106365   -16.986885    -1.252969
C     93    -0.459981   -17.668469    -2.465095
C     94    -0.379862   -19.194888    -2.339188
C     95     0.267059   -19.868134    -3.553176
H     96    -1.262358   -15.057935     0.742907
H     97    -2.842032   -15.195725    -0.010022
H     98    -0.177284   -15.052068    -1.529715
H     99    -1.757602   -15.192212    -2.280054
H    100    -0.541104   -17.245737    -0.346205
H    101    -2.117622   -17.392114    -1.104985
H    102     0.551382   -17.263738    -2.612984
H    103    -1.024619   -17.408970    -3.371911
H    104     0.184409   -19.453608    -1.432889
H    105    -1.390691   -19.598876    -2.191702
H    106     1.291676   -19.510428    -3.705605
H    107    -0.295011   -19.656885    -4.469956
H    108     0.309484   -20.955440    -3.432876
S    109     1.874349     8.046436    -0.334048
C    110    -0.680277     7.784383    -0.609660
C    111    -0.432838     9.175198    -0.596662
C    112     0.902925     9.503316    -0.463476
H    113    -1.211730     9.921640    -0.702227
H    114    -1.670077     7.356711    -0.723230
S    115     0.548998    12.258924    -0.195891
C    116     1.958214    13.296310    -0.261058
C    117     3.092289    12.544942    -0.434738
C    118     2.851485    11.146903    -0.524729
C    119     1.519348    10.809015    -0.418959
H    120     3.634376    10.412224    -0.677154
H    121     4.080192    12.988187    -0.499658
C    122     1.833830    14.789187    -0.155754
C    123     1.185281    15.461515    -1.383264
C    124     1.106365    16.986885    -1.252969
C    125     0.459981    17.668469    -2.465095
C    126     0.379862    19.194888    -2.339188
C    127    -0.267059    19.868134    -3.553176
H    128     1.262358    15.057935     0.742907
H    129     2.842032    15.195725    -0.010022
H    130     0.177284    15.052068    -1.529715
H    131     1.757602    15.192212    -2.280054
H    132     0.541104    17.245737    -0.346205
H    133     2.117622    17.392114    -1.104985
H    134    -0.551382    17.263738    -2.612984
H    135     1.024619    17.408970    -3.371911
H    136    -0.184409    19.453608    -1.432889
H    137     1.390691    19.598876    -2.191702
H    138    -1.291676    19.510428    -3.705605
H    139     0.295011    19.656885    -4.469956
H    140    -0.309484    20.955440    -3.432876
```

T3-A

C	1	0.412732	0.576627	0.089140
C	2	-0.412732	-0.576627	0.089140
C	3	1.791597	0.145575	0.055094
C	4	-1.791597	-0.145575	0.055094
C	5	0.388101	-1.723277	0.035901
C	6	-0.388101	1.723277	0.035901
N	7	1.715612	-1.285291	0.044400
N	8	-1.715612	1.285291	0.044400
O	9	2.862456	0.753589	0.048666
O	10	-2.862456	-0.753589	0.048666
C	11	-0.074870	-3.078494	-0.069938
C	12	0.074870	3.078494	-0.069938
S	13	0.934155	-4.490262	-0.390429
S	14	-0.934155	4.490262	-0.390429
C	15	-0.450280	-5.563006	-0.397584
C	16	0.450280	5.563006	-0.397584
C	17	-1.614142	-4.843197	-0.174548
C	18	1.614142	4.843197	-0.174548
C	19	-1.410626	-3.464815	0.003581
C	20	1.410626	3.464815	0.003581
C	21	-0.287816	-6.976271	-0.616549
C	22	0.287816	6.976271	-0.616549
H	23	-2.592132	-5.308897	-0.131551
H	24	2.592132	5.308897	-0.131551
H	25	-2.204696	-2.744267	0.169983
H	26	2.204696	2.744267	0.169983
C	27	2.947640	-2.065742	0.140203
C	28	-2.947640	2.065742	0.140203
C	29	3.235837	-2.669047	1.535527
C	30	-3.235837	2.669047	1.535527
C	31	4.449454	-3.614330	1.417157
C	32	-4.449454	3.614330	1.417157
C	33	4.790319	-4.392037	2.694831
C	34	-4.790319	4.392037	2.694831
C	35	5.922200	-5.408551	2.496206
C	36	-5.922200	5.408551	2.496206
C	37	6.269435	-6.182691	3.771242
C	38	-6.269435	6.182691	3.771242
C	39	3.376077	-1.600067	2.643230
C	40	-3.376077	1.600067	2.643230
C	41	4.608170	-0.690095	2.560548
C	42	-4.608170	0.690095	2.560548
H	43	3.741177	-1.370107	-0.143160
H	44	-3.741177	1.370107	-0.143160
H	45	2.933660	-2.855663	-0.616702
H	46	-2.933660	2.855663	-0.616702
H	47	7.078292	-6.899731	3.597127
H	48	-7.078292	6.899731	3.597127
H	49	2.370737	-3.288810	1.807855

```
H      50    -2.370737     3.288810     1.807855
H      51     5.331491    -3.046550     1.090577
H      52    -5.331491     3.046550     1.090577
H      53     4.246472    -4.337003     0.614099
H      54    -4.246472     4.337003     0.614099
H      55     5.074470    -3.696065     3.494514
H      56    -5.074470     3.696065     3.494514
H      57     3.892019    -4.915776     3.052098
H      58    -3.892019     4.915776     3.052098
H      59     6.816676    -4.886555     2.129841
H      60    -6.816676     4.886555     2.129841
H      61     5.639475    -6.115405     1.704092
H      62    -5.639475     6.115405     1.704092
H      63     6.591961    -5.505706     4.570427
H      64    -6.591961     5.505706     4.570427
H      65     5.403592    -6.742029     4.143497
H      66    -5.403592     6.742029     4.143497
H      67     3.371338    -2.114648     3.611569
H      68    -3.371338     2.114648     3.611569
H      69     2.472221    -0.978948     2.639802
H      70    -2.472221     0.978948     2.639802
H      71     5.542990    -1.258827     2.608728
H      72    -5.542990     1.258827     2.608728
H      73     4.607521    -0.097254     1.642341
H      74    -4.607521     0.097254     1.642341
H      75     4.612672     0.011702     3.401137
H      76    -4.612672    -0.011702     3.401137
S      77    -1.686810    -8.022338    -0.823243
C      78     0.875355    -7.718753    -0.704014
C      79     0.658328    -9.098507    -0.915518
C      80    -0.676398    -9.447696    -0.996403
H      81     1.459446    -9.825140    -0.987599
H      82     1.861315    -7.279931    -0.600075
S      83    -0.282528   -12.118461    -1.705150
C      84    -1.660069   -13.199458    -1.701692
C      85    -2.794532   -12.520567    -1.336978
C      86    -2.578490   -11.144966    -1.051573
C      87    -1.265459   -10.751373    -1.196765
H      88    -3.364148   -10.467714    -0.735375
H      89    -3.765031   -13.000742    -1.272290
C      90    -1.511214   -14.654465    -2.042263
C      91    -0.758841   -15.482458    -0.980296
C      92    -0.658328   -16.967676    -1.346336
C      93     0.091044   -17.802647    -0.300937
C      94     0.192478   -19.289626    -0.662647
C      95     0.942386   -20.116680     0.385755
H      96    -2.518339   -15.067282    -2.177368
H      97    -1.002335   -14.765709    -3.009238
H      98    -1.267974   -15.369210    -0.014749
H      99     0.248581   -15.067784    -0.844983
H     100    -1.669245   -17.378012    -1.482062
```

```
H    101    -0.157417    -17.069359    -2.319724
H    102    -0.409038    -17.699993     0.672646
H    103     1.102214    -17.393044    -0.165678
H    104    -0.818168    -19.698498    -0.797382
H    105     0.692133    -19.391607    -1.635607
H    106     0.446708    -20.063059     1.361699
H    107     1.968118    -19.753913     0.517285
H    108     0.997634    -21.171770     0.098991
S    109     1.686810      8.022338    -0.823243
C    110    -0.875355      7.718753    -0.704014
C    111    -0.658328      9.098507    -0.915518
C    112     0.676398      9.447696    -0.996403
H    113    -1.459446      9.825140    -0.987599
H    114    -1.861315      7.279931    -0.600075
S    115     0.282528     12.118461    -1.705150
C    116     1.660069     13.199458    -1.701692
C    117     2.794532     12.520567    -1.336978
C    118     2.578490     11.144966    -1.051573
C    119     1.265459     10.751373    -1.196765
H    120     3.364148     10.467714    -0.735375
H    121     3.765031     13.000742    -1.272290
C    122     1.511214     14.654465    -2.042263
C    123     0.758841     15.482458    -0.980296
C    124     0.658328     16.967676    -1.346336
C    125    -0.091044     17.802647    -0.300937
C    126    -0.192478     19.289626    -0.662647
C    127    -0.942386     20.116680     0.385755
H    128     1.002335     14.765709    -3.009238
H    129     2.518339     15.067282    -2.177368
H    130    -0.248581     15.067784    -0.844983
H    131     1.267974     15.369210    -0.014749
H    132     0.157417     17.069359    -2.319724
H    133     1.669245     17.378012    -1.482062
H    134    -1.102214     17.393044    -0.165678
H    135     0.409038     17.699993     0.672646
H    136    -0.692133     19.391607    -1.635607
H    137     0.818168     19.698498    -0.797382
H    138    -1.968118     19.753913     0.517285
H    139    -0.446708     20.063059     1.361699
H    140    -0.997634     21.171770     0.098991
```

b) Neutral molecule in dichloromethane calculated by PCM/B3LYP/6-31++G(d,p) method

T1-B
```
C      1    -0.711628     -0.005222    -1.336604
C      2     0.711628      0.005222    -1.336604
C      3    -1.166753      1.362979    -1.348799
C      4     1.166753     -1.362979    -1.348799
C      5     1.166753      1.329199    -1.353871
C      6    -1.166753     -1.329199    -1.353871
N      7     0.032228      2.141015    -1.361366
```

```
N     8    -0.032228    -2.141015    -1.361366
O     9    -2.291141     1.880164    -1.348239
O    10     2.291141    -1.880164    -1.348239
C    11     2.541763     1.768213    -1.377518
C    12    -2.541763    -1.768213    -1.377518
S    13     3.097882     3.438956    -1.464820
S    14    -3.097882    -3.438956    -1.464820
C    15     4.752756     2.949944    -1.450130
C    16    -4.752756    -2.949944    -1.450130
C    17     4.885313     1.584040    -1.383756
C    18    -4.885313    -1.584040    -1.383756
C    19     3.639101     0.912224    -1.343401
C    20    -3.639101    -0.912224    -1.343401
H    21     5.529955     3.701262    -1.493306
H    22    -5.529955    -3.701262    -1.493306
H    23     5.843481     1.078324    -1.363983
H    24    -5.843481    -1.078324    -1.363983
H    25     3.524489    -0.164996    -1.295152
H    26    -3.524489     0.164996    -1.295152
C    27    -0.069138     3.600737    -1.303848
C    28     0.069138    -3.600737    -1.303848
C    29    -0.008944     4.164650     0.123201
C    30     0.008944    -4.164650     0.123201
C    31    -0.151690     5.691895     0.144126
C    32     0.151690    -5.691895     0.144126
C    33    -0.128367     6.280275     1.561255
C    34     0.128367    -6.280275     1.561255
C    35    -0.272339     7.807643     1.591694
C    36     0.272339    -7.807643     1.591694
C    37    -0.253513     8.397231     3.008144
C    38     0.253513    -8.397231     3.008144
C    39    -0.397863     9.924615     3.041631
C    40     0.397863    -9.924615     3.041631
C    41    -0.378675    10.504617     4.460792
C    42     0.378675   -10.504617     4.460792
H    43    -1.035445     3.843756    -1.752203
H    44     1.035445    -3.843756    -1.752203
H    45     0.698186     4.041446    -1.943768
H    46    -0.698186    -4.041446    -1.943768
H    47    -0.814426     3.707596     0.711109
H    48     0.814426    -3.707596     0.711109
H    49     0.935776     3.874864     0.599307
H    50    -0.935776    -3.874864     0.599307
H    51    -1.091660     5.975463    -0.350301
H    52     1.091660    -5.975463    -0.350301
H    53     0.657131     6.142201    -0.449004
H    54    -0.657131    -6.142201    -0.449004
H    55    -0.937452     5.828251     2.152667
H    56     0.937452    -5.828251     2.152667
H    57     0.810894     5.994614     2.056359
H    58    -0.810894    -5.994614     2.056359
```

```
H    59   -1.210677     8.092421     1.093868
H    60    1.210677    -8.092421     1.093868
H    61    0.537708     8.259590     1.000837
H    62   -0.537708    -8.259590     1.000837
H    63   -1.063562     7.945586     3.599445
H    64    1.063562    -7.945586     3.599445
H    65    0.684657     8.112749     3.506968
H    66   -0.684657    -8.112749     3.506968
H    67   -1.335164    10.209220     2.543533
H    68    1.335164   -10.209220     2.543533
H    69    0.411616    10.376503     2.451512
H    70   -0.411616   -10.376503     2.451512
H    71   -1.197923    10.097059     5.065306
H    72    1.197923   -10.097059     5.065306
H    73    0.561266    10.265558     4.972761
H    74   -0.561266   -10.265558     4.972761
H    75   -0.483753    11.595128     4.449137
H    76    0.483753   -11.595128     4.449137

T1-A
C     1   -0.709376     0.057753    -0.817028
C     2    0.709376    -0.057753    -0.817028
C     3   -1.045039     1.461368    -0.874183
C     4    1.045039    -1.461368    -0.874183
C     5    1.274710     1.216254    -0.901765
C     6   -1.274710    -1.216254    -0.901765
N     7    0.218930     2.131412    -0.903670
N     8   -0.218930    -2.131412    -0.903670
O     9   -2.123134     2.065198    -0.882458
O    10    2.123134    -2.065198    -0.882458
C    11    2.679194     1.528675    -1.024767
C    12   -2.679194    -1.528675    -1.024767
S    13    3.341967     3.064835    -1.575146
S    14   -3.341967    -3.064835    -1.575146
C    15    4.958639     2.466377    -1.477321
C    16   -4.958639    -2.466377    -1.477321
C    17    4.999582     1.161210    -1.050115
C    18   -4.999582    -1.161210    -1.050115
C    19    3.711813     0.624876    -0.800139
C    20   -3.711813    -0.624876    -0.800139
H    21    5.783175     3.114950    -1.741615
H    22   -5.783175    -3.114950    -1.741615
H    23    5.920247     0.604554    -0.920899
H    24   -5.920247    -0.604554    -0.920899
H    25    3.524577    -0.395395    -0.487604
H    26   -3.524577     0.395395    -0.487604
C    27    0.273924     3.591905    -0.788077
C    28   -0.273924    -3.591905    -0.788077
C    29    0.728565     4.117347     0.594365
C    30   -0.728565    -4.117347     0.594365
C    31    0.952108     5.640765     0.490477
```

```
C    32    -0.952108    -5.640765     0.490477
C    33     1.540203     6.293290     1.749440
C    34    -1.540203    -6.293290     1.749440
C    35     1.858372     7.783184     1.560981
C    36    -1.858372    -7.783184     1.560981
C    37     2.439696     8.440804     2.818040
C    38    -2.439696    -8.440804     2.818040
C    39    -0.218930     3.695420     1.741678
C    40     0.218930    -3.695420     1.741678
C    41    -1.604945     4.355890     1.756305
C    42     1.604945    -4.355890     1.756305
H    43    -0.740174     3.931582    -1.010066
H    44     0.740174    -3.931582    -1.010066
H    45     0.917184     3.991274    -1.576506
H    46    -0.917184    -3.991274    -1.576506
H    47     2.657405     9.501269     2.650003
H    48    -2.657405    -9.501269     2.650003
H    49     1.704646     3.663685     0.813257
H    50    -1.704646    -3.663685     0.813257
H    51     0.007497     6.137919     0.229799
H    52    -0.007497    -6.137919     0.229799
H    53     1.634345     5.831315    -0.349764
H    54    -1.634345    -5.831315    -0.349764
H    55     0.844844     6.183484     2.591929
H    56    -0.844844    -6.183484     2.591929
H    57     2.458925     5.761639     2.037518
H    58    -2.458925    -5.761639     2.037518
H    59     0.942962     8.312512     1.262021
H    60    -0.942962    -8.312512     1.262021
H    61     2.565095     7.899149     0.727617
H    62    -2.565095    -7.899149     0.727617
H    63     1.739620     8.373226     3.659402
H    64    -1.739620    -8.373226     3.659402
H    65     3.373104     7.952914     3.123615
H    66    -3.373104    -7.952914     3.123615
H    67     0.285485     3.903524     2.692875
H    68    -0.285485    -3.903524     2.692875
H    69    -0.340172     2.605305     1.708739
H    70     0.340172    -2.605305     1.708739
H    71    -1.538653     5.441809     1.882686
H    72     1.538653    -5.441809     1.882686
H    73    -2.161751     4.152174     0.836641
H    74     2.161751    -4.152174     0.836641
H    75    -2.198189     3.965977     2.590699
H    76     2.198189    -3.965977     2.590699


T2-B
C     1    -0.396792    -0.589502    -0.198191
C     2     0.396792     0.589502    -0.198191
C     3    -1.783153    -0.194834    -0.213944
C     4     1.783153     0.194834    -0.213944
```

```
C      5     -0.440756     1.715223    -0.224813
C      6      0.440756    -1.715223    -0.224813
N      7     -1.751745     1.232377    -0.233039
N      8      1.751745    -1.232377    -0.233039
O      9     -2.843612    -0.835447    -0.208216
O     10      2.843612     0.835447    -0.208216
C     11     -0.029590     3.091097    -0.262371
C     12      0.029590    -3.091097    -0.262371
S     13     -1.096147     4.490151    -0.406948
S     14      1.096147    -4.490151    -0.406948
C     15      0.249660     5.608717    -0.384544
C     16     -0.249660    -5.608717    -0.384544
C     17      1.448100     4.917057    -0.274364
C     18     -1.448100    -4.917057    -0.274364
C     19      1.295938     3.520310    -0.208539
C     20     -1.295938    -3.520310    -0.208539
C     21      0.029590     7.033059    -0.477094
C     22     -0.029590    -7.033059    -0.477094
H     23      2.412590     5.410674    -0.240509
H     24     -2.412590    -5.410674    -0.240509
H     25      2.120088     2.819868    -0.129404
H     26     -2.120088    -2.819868    -0.129404
C     27     -3.012759     1.972242    -0.157556
C     28      3.012759    -1.972242    -0.157556
C     29     -3.412447     2.360520     1.273402
C     30      3.412447    -2.360520     1.273402
C     31     -4.753916     3.103458     1.314368
C     32      4.753916    -3.103458     1.314368
C     33     -5.191712     3.479822     2.736237
C     34      5.191712    -3.479822     2.736237
C     35     -6.533620     4.222192     2.786916
C     36      6.533620    -4.222192     2.786916
C     37     -6.973759     4.596944     4.208260
C     38      6.973759    -4.596944     4.208260
C     39     -8.315779     5.339122     4.262134
C     40      8.315779    -5.339122     4.262134
C     41     -8.747430     5.709197     5.686052
C     42      8.747430    -5.709197     5.686052
H     43     -3.767622     1.304802    -0.580010
H     44      3.767622    -1.304802    -0.580010
H     45     -2.959995     2.845797    -0.811142
H     46      2.959995    -2.845797    -0.811142
H     47     -3.474762     1.446351     1.876606
H     48      3.474762    -1.446351     1.876606
H     49     -2.630207     2.984894     1.722228
H     50      2.630207    -2.984894     1.722228
H     51     -5.529583     2.478173     0.849852
H     52      5.529583    -2.478173     0.849852
H     53     -4.685136     4.014742     0.703046
H     54      4.685136    -4.014742     0.703046
H     55     -5.259145     2.567543     3.346092
```

```
H     56     5.259145    -2.567543     3.346092
H     57    -4.414528     4.103475     3.200937
H     58     4.414528    -4.103475     3.200937
H     59    -7.309938     3.598348     2.320486
H     60     7.309938    -3.598348     2.320486
H     61    -6.465885     5.134746     2.176775
H     62     6.465885    -5.134746     2.176775
H     63    -7.041612     3.684667     4.818959
H     64     7.041612    -3.684667     4.818959
H     65    -6.197739     5.220912     4.675545
H     66     6.197739    -5.220912     4.675545
H     67    -9.091510     4.715902     3.795797
H     68     9.091510    -4.715902     3.795797
H     69    -8.248430     6.250967     3.652427
H     70     8.248430    -6.250967     3.652427
H     71    -8.856650     4.814578     6.310910
H     72     8.856650    -4.814578     6.310910
H     73    -8.007392     6.360416     6.166687
H     74     8.007392    -6.360416     6.166687
H     75    -9.707593     6.236912     5.689012
H     76     9.707593    -6.236912     5.689012
S     77     1.382333     8.158458    -0.504241
C     78     0.319493     9.544142    -0.616779
C     79    -0.994526     9.137642    -0.631467
C     80    -1.162834     7.728146    -0.553956
H     81    -2.132749     7.242769    -0.550888
H     82    -1.820684     9.837817    -0.693814
C     83     0.863580    10.941497    -0.706746
C     84     1.543488    11.272903    -2.052659
C     85     2.039900    12.722390    -2.122583
C     86     2.716963    13.068759    -3.455257
C     87     3.213776    14.518646    -3.532470
C     88     3.889065    14.856790    -4.866740
H     89     0.026190    11.630600    -0.544565
H     90     1.577404    11.119899     0.108187
H     91     0.831548    11.084708    -2.866954
H     92     2.387226    10.588604    -2.211861
H     93     1.192713    13.403880    -1.958541
H     94     2.745276    12.904366    -1.298937
H     95     2.011880    12.884585    -4.278891
H     96     3.564672    12.387636    -3.619234
H     97     2.366753    15.199320    -3.368837
H     98     3.918212    14.702919    -2.709473
H     99     3.198303    14.714550    -5.706537
H    100     4.760749    14.214965    -5.042383
H    101     4.231357    15.897277    -4.889323
S    102    -1.382333    -8.158458    -0.504241
C    103    -0.319493    -9.544142    -0.616779
C    104     0.994526    -9.137642    -0.631467
C    105     1.162834    -7.728146    -0.553956
H    106     2.132749    -7.242769    -0.550888
```

```
H    107     1.820684    -9.837817    -0.693814
C    108    -0.863580   -10.941497    -0.706746
C    109    -1.543488   -11.272903    -2.052659
C    110    -2.039900   -12.722390    -2.122583
C    111    -2.716963   -13.068759    -3.455257
C    112    -3.213776   -14.518646    -3.532470
C    113    -3.889065   -14.856790    -4.866740
H    114    -1.577404   -11.119899     0.108187
H    115    -0.026190   -11.630600    -0.544565
H    116    -2.387226   -10.588604    -2.211861
H    117    -0.831548   -11.084708    -2.866954
H    118    -2.745276   -12.904366    -1.298937
H    119    -1.192713   -13.403880    -1.958541
H    120    -3.564672   -12.387636    -3.619234
H    121    -2.011880   -12.884585    -4.278891
H    122    -3.918212   -14.702919    -2.709473
H    123    -2.366753   -15.199320    -3.368837
H    124    -4.760749   -14.214965    -5.042383
H    125    -3.198303   -14.714550    -5.706537
H    126    -4.231357   -15.897277    -4.889323

T2-A
C      1    -0.376718    -0.602686    -0.314872
C      2     0.376718     0.602686    -0.314872
C      3    -1.777302    -0.257339    -0.372518
C      4     1.777302     0.257339    -0.372518
C      5    -0.496834     1.693642    -0.400278
C      6     0.496834    -1.693642    -0.400278
N      7    -1.794734     1.171392    -0.401641
N      8     1.794734    -1.171392    -0.401641
O      9    -2.808664    -0.940596    -0.381188
O     10     2.808664     0.940596    -0.381188
C     11    -0.131952     3.077606    -0.530095
C     12     0.131952    -3.077606    -0.530095
S     13    -1.206688     4.375612    -1.050746
S     14     1.206688    -4.375612    -1.050746
C     15     0.079147     5.561848    -0.984315
C     16    -0.079147    -5.561848    -0.984315
C     17     1.265911     4.963347    -0.584377
C     18    -1.265911    -4.963347    -0.584377
C     19     1.152281     3.582165    -0.338997
C     20    -1.152281    -3.582165    -0.338997
C     21    -0.170944     6.943835    -1.322379
C     22     0.170944    -6.943835    -1.322379
H     23     2.194236     5.511532    -0.471383
H     24    -2.194236    -5.511532    -0.471383
H     25     1.979638     2.945875    -0.047940
H     26    -1.979638    -2.945875    -0.047940
C     27    -3.066388     1.888778    -0.273864
C     28     3.066388    -1.888778    -0.273864
C     29    -3.316011     2.525288     1.114360
```

```
C    30     3.316011    -2.525288     1.114360
C    31    -4.569347     3.421306     1.025420
C    32     4.569347    -3.421306     1.025420
C    33    -4.869820     4.236907     2.290796
C    34     4.869820    -4.236907     2.290796
C    35    -6.051250     5.201590     2.117410
C    36     6.051250    -5.201590     2.117410
C    37    -6.359223     6.013358     3.381054
C    38     6.359223    -6.013358     3.381054
C    39    -3.365647     1.483143     2.256038
C    40     3.365647    -1.483143     2.256038
C    41    -4.586689     0.552631     2.273004
C    42     4.586689    -0.552631     2.273004
H    43    -3.834837     1.145157    -0.496630
H    44     3.834837    -1.145157    -0.496630
H    45    -3.131239     2.649406    -1.056545
H    46     3.131239    -2.649406    -1.056545
H    47    -7.204776     6.692050     3.223949
H    48     7.204776    -6.692050     3.223949
H    49    -2.464523     3.184573     1.330641
H    50     2.464523    -3.184573     1.330641
H    51    -5.445934     2.810127     0.769522
H    52     5.445934    -2.810127     0.769522
H    53    -4.434073     4.119037     0.187197
H    54     4.434073    -4.119037     0.187197
H    55    -5.082546     3.564283     3.132071
H    56     5.082546    -3.564283     3.132071
H    57    -3.974540     4.809752     2.573563
H    58     3.974540    -4.809752     2.573563
H    59    -6.943096     4.630626     1.823816
H    60     6.943096    -4.630626     1.823816
H    61    -5.838859     5.887113     1.285326
H    62     5.838859    -5.887113     1.285326
H    63    -6.611032     5.355804     4.221765
H    64     6.611032    -5.355804     4.221765
H    65    -5.496108     6.619524     3.681439
H    66     5.496108    -6.619524     3.681439
H    67    -3.313256     2.021161     3.210159
H    68     3.313256    -2.021161     3.210159
H    69    -2.451918     0.877088     2.212768
H    70     2.451918    -0.877088     2.212768
H    71    -5.521134     1.107376     2.409630
H    72     5.521134    -1.107376     2.409630
H    73    -4.665796    -0.028728     1.349423
H    74     4.665796     0.028728     1.349423
H    75    -4.505599    -0.159304     3.101724
H    76     4.505599     0.159304     3.101724
S    77     1.128070     8.130851    -1.299733
C    78     0.054595     9.420492    -1.796751
C    79    -1.222860     8.939361    -1.965365
C    80    -1.355024     7.548867    -1.699985
```

```
H      81    -2.293480    7.012148    -1.786758
H      82    -2.047692    9.571911    -2.275503
C      83     0.549857   10.828797    -1.964359
C      84     0.896483   11.542723    -0.640122
C      85     1.355024   12.990849    -0.852347
C      86     1.701686   13.715909     0.454755
C      87     2.160421   15.165813     0.249091
C      88     2.505190   15.883152     1.559501
H      89     1.431320   10.841365    -2.618844
H      90    -0.233574   11.392066    -2.485337
H      91     1.684075   10.981681    -0.120075
H      92     0.015929   11.524311     0.015374
H      93     2.231673   13.000039    -1.516021
H      94     0.565656   13.547799    -1.377473
H      95     2.491039   13.158859     0.980175
H      96     0.825105   13.705442     1.118790
H      97     3.036220   15.176331    -0.414515
H      98     1.371778   15.722692    -0.275750
H      99     3.314820   15.368388     2.090670
H     100     1.638568   15.918427     2.230594
H     101     2.828337   16.914128     1.378008
S     102    -1.128070   -8.130851    -1.299733
C     103    -0.054595   -9.420492    -1.796751
C     104     1.222860   -8.939361    -1.965365
C     105     1.355024   -7.548867    -1.699985
H     106     2.293480   -7.012148    -1.786758
H     107     2.047692   -9.571911    -2.275503
C     108    -0.549857  -10.828797    -1.964359
C     109    -0.896483  -11.542723    -0.640122
C     110    -1.355024  -12.990849    -0.852347
C     111    -1.701686  -13.715909     0.454755
C     112    -2.160421  -15.165813     0.249091
C     113    -2.505190  -15.883152     1.559501
H     114     0.233574  -11.392066    -2.485337
H     115    -1.431320  -10.841365    -2.618844
H     116    -0.015929  -11.524311     0.015374
H     117    -1.684075  -10.981681    -0.120075
H     118    -0.565656  -13.547799    -1.377473
H     119    -2.231673  -13.000039    -1.516021
H     120    -0.825105  -13.705442     1.118790
H     121    -2.491039  -13.158859     0.980175
H     122    -1.371778  -15.722692    -0.275750
H     123    -3.036220  -15.176331    -0.414515
H     124    -1.638568  -15.918427     2.230594
H     125    -3.314820  -15.368388     2.090670
H     126    -2.828337  -16.914128     1.378008


T2-D
C       1     0.651156   -0.285735    -0.252047
C       2    -0.651156    0.285735    -0.252047
C       3     1.611257    0.790265    -0.281400
```

```
C      4    -1.611257    -0.790265    -0.281400
C      5    -0.545645     1.682151    -0.300777
C      6     0.545645    -1.682151    -0.300777
N      7     0.819249     1.978469    -0.315485
N      8    -0.819249    -1.978469    -0.315485
O      9     2.849004     0.816628    -0.269434
O     10    -2.849004    -0.816628    -0.269434
C     11    -1.630385     2.626315    -0.351809
C     12     1.630385    -2.626315    -0.351809
S     13    -1.483181     4.359740    -0.630077
S     14     1.483181    -4.359740    -0.630077
C     15    -3.217444     4.589623    -0.601796
C     16     3.217444    -4.589623    -0.601796
C     17    -3.853980     3.379357    -0.365297
C     18     3.853980    -3.379357    -0.365297
C     19    -2.976581     2.286883    -0.232359
C     20     2.976581    -2.286883    -0.232359
C     21    -3.832870     5.898043    -0.748023
C     22     3.832870    -5.898043    -0.748023
H     23    -4.932695     3.287241    -0.314330
H     24     4.932695    -3.287241    -0.314330
H     25    -3.297141     1.262354    -0.080276
H     26     3.297141    -1.262354    -0.080276
C     27     1.483181     3.279620    -0.212433
C     28    -1.483181    -3.279620    -0.212433
C     29     1.556366     3.817858     1.223900
C     30    -1.556366    -3.817858     1.223900
C     31     2.288430     5.163918     1.297486
C     32    -2.288430    -5.163918     1.297486
C     33     2.405136     5.710204     2.726877
C     34    -2.405136    -5.710204     2.726877
C     35     3.138261     7.055728     2.808738
C     36    -3.138261    -7.055728     2.808738
C     37     3.260162     7.602422     4.237255
C     38    -3.260162    -7.602422     4.237255
C     39     3.993618     8.947781     4.321079
C     40    -3.993618    -8.947781     4.321079
C     41     4.111721     9.486112     5.751837
C     42    -4.111721    -9.486112     5.751837
H     43     0.996630     3.990884    -0.883432
H     44    -0.996630    -3.990884    -0.883432
H     45     2.493122     3.120547    -0.597401
H     46    -2.493122    -3.120547    -0.597401
H     47     0.544332     3.924910     1.633352
H     48    -0.544332    -3.924910     1.633352
H     49     2.074497     3.077779     1.846347
H     50    -2.074497    -3.077779     1.846347
H     51     1.763698     5.898994     0.670598
H     52    -1.763698    -5.898994     0.670598
H     53     3.294541     5.054116     0.868405
H     54    -3.294541    -5.054116     0.868405
```

```
H      55      1.398733      5.818720      3.156070
H      56     -1.398733     -5.818720      3.156070
H      57      2.928692      4.973585      3.352943
H      58     -2.928692     -4.973585      3.352943
H      59      2.613535      7.792477      2.183237
H      60     -2.613535     -7.792477      2.183237
H      61      4.143541      6.946608      2.376375
H      62     -4.143541     -6.946608      2.376375
H      63      2.255146      7.712049      4.670561
H      64     -2.255146     -7.712049      4.670561
H      65      3.784887      6.866121      4.863591
H      66     -3.784887     -6.866121      4.863591
H      67      3.469201      9.684004      3.696072
H      68     -3.469201     -9.684004      3.696072
H      69      4.997714      8.838693      3.888012
H      70     -4.997714     -8.838693      3.888012
H      71      3.122290      9.637963      6.199825
H      72     -3.122290     -9.637963      6.199825
H      73      4.661710      8.786763      6.393029
H      74     -4.661710     -8.786763      6.393029
H      75      4.639415     10.445977      5.776197
H      76     -4.639415    -10.445977      5.776197
S      77     -5.303067      6.221502      0.169089
C      78     -5.442131      7.804928     -0.512450
C      79     -4.418995      8.069377     -1.381544
C      80     -3.486456      6.991917     -1.531645
H      81     -6.268271      8.444737     -0.232764
H      82     -4.328415      9.005358     -1.922513
C      83     -2.310135      7.091120     -2.472869
C      84     -1.122498      7.895462     -1.902293
C      85      0.040766      8.020272     -2.894449
C      86      1.228377      8.821030     -2.344235
C      87      2.392879      8.951695     -3.335252
C      88      3.573814      9.756014     -2.779157
H      89     -1.966953      6.092047     -2.760922
H      90     -2.650272      7.579125     -3.395431
H      91     -0.769462      7.417967     -0.978628
H      92     -1.470413      8.897133     -1.616846
H      93      0.382313      7.015379     -3.181710
H      94     -0.321270      8.496350     -3.817181
H      95      1.591508      8.344402     -1.422065
H      96      0.885880      9.825513     -2.055667
H      97      2.736814      7.948205     -3.621944
H      98      2.029858      9.426029     -4.257594
H      99      3.980052      9.287701     -1.874609
H     100      3.268232     10.775761     -2.515683
H     101      4.386685      9.829980     -3.509939
S     102      5.303067     -6.221502      0.169089
C     103      5.442131     -7.804928     -0.512450
C     104      4.418995     -8.069377     -1.381544
C     105      3.486456     -6.991917     -1.531645
```

```
H    106    6.268271    -8.444737    -0.232764
H    107    4.328415    -9.005358    -1.922513
C    108    2.310135    -7.091120    -2.472869
C    109    1.122498    -7.895462    -1.902293
C    110   -0.040766    -8.020272    -2.894449
C    111   -1.228377    -8.821030    -2.344235
C    112   -2.392879    -8.951695    -3.335252
C    113   -3.573814    -9.756014    -2.779157
H    114    1.966953    -6.092047    -2.760922
H    115    2.650272    -7.579125    -3.395431
H    116    0.769462    -7.417967    -0.978628
H    117    1.470413    -8.897133    -1.616846
H    118   -0.382313    -7.015379    -3.181710
H    119    0.321270    -8.496350    -3.817181
H    120   -1.591508    -8.344402    -1.422065
H    121   -0.885880    -9.825513    -2.055667
H    122   -2.736814    -7.948205    -3.621944
H    123   -2.029858    -9.426029    -4.257594
H    124   -3.980052    -9.287701    -1.874609
H    125   -3.268232   -10.775761    -2.515683
H    126   -4.386685    -9.829980    -3.509939

T2-C
C      1   -0.616141    -0.355172     0.427513
C      2    0.616141     0.355172     0.427513
C      3   -1.690423     0.608462     0.367238
C      4    1.690423    -0.608462     0.367238
C      5    0.357338     1.726247     0.336795
C      6   -0.357338    -1.726247     0.336795
N      7   -1.032935     1.877464     0.334544
N      8    1.032935    -1.877464     0.334544
O      9   -2.921176     0.490499     0.360538
O     10    2.921176    -0.490499     0.360538
C     11    1.330562     2.779279     0.207675
C     12   -1.330562    -2.779279     0.207675
S     13    0.998025     4.415869    -0.349316
S     14   -0.998025    -4.415869    -0.349316
C     15    2.690935     4.856719    -0.301885
C     16   -2.690935    -4.856719    -0.301885
C     17    3.450156     3.784352     0.144188
C     18   -3.450156    -3.784352     0.144188
C     19    2.698126     2.625447     0.418057
C     20   -2.698126    -2.625447     0.418057
C     21    3.156663     6.193203    -0.633763
C     22   -3.156663    -6.193203    -0.633763
H     23    4.528238     3.833595     0.244338
H     24   -4.528238    -3.833595     0.244338
H     25    3.127960     1.680124     0.727319
H     26   -3.127960    -1.680124     0.727319
C     27   -1.815286     3.109550     0.472245
C     28    1.815286    -3.109550     0.472245
```

```
C     29    -1.721273     3.785768     1.860819
C     30     1.721273    -3.785768     1.860819
C     31    -2.406239     5.166366     1.780434
C     32     2.406239    -5.166366     1.780434
C     33    -2.279486     6.024610     3.046938
C     34     2.279486    -6.024610     3.046938
C     35    -2.868897     7.432178     2.879768
C     36     2.868897    -7.432178     2.879768
C     37    -2.751902     8.290666     4.144687
C     38     2.751902    -8.290666     4.144687
C     39    -2.243278     2.887611     3.006483
C     40     2.243278    -2.887611     3.006483
C     41    -3.757784     2.637314     3.037533
C     42     3.757784    -2.637314     3.037533
H     43    -2.845699     2.816323     0.259351
H     44     2.845699    -2.816323     0.259351
H     45    -1.521936     3.812753    -0.311619
H     46     1.521936    -3.812753    -0.311619
H     47    -3.179537     9.287687     3.991954
H     48     3.179537    -9.287687     3.991954
H     49    -0.657534     3.966727     2.066468
H     50     0.657534    -3.966727     2.066468
H     51    -3.468956     5.040088     1.531049
H     52     3.468956    -5.040088     1.531049
H     53    -1.963575     5.720351     0.940876
H     54     1.963575    -5.720351     0.940876
H     55    -2.778523     5.529553     3.890286
H     56     2.778523    -5.529553     3.890286
H     57    -1.218197     6.108112     3.323117
H     58     1.218197    -6.108112     3.323117
H     59    -3.926089     7.348669     2.591722
H     60     3.926089    -7.348669     2.591722
H     61    -2.363343     7.938956     2.046229
H     62     2.363343    -7.938956     2.046229
H     63    -3.278866     7.827088     4.987284
H     64     3.278866    -7.827088     4.987284
H     65    -1.703449     8.418951     4.439492
H     66     1.703449    -8.418951     4.439492
H     67    -1.936151     3.337796     3.958057
H     68     1.936151    -3.337796     3.958057
H     69    -1.720441     1.924078     2.958079
H     70     1.720441    -1.924078     2.958079
H     71    -4.322491     3.565707     3.174707
H     72     4.322491    -3.565707     3.174707
H     73    -4.108438     2.156089     2.119531
H     74     4.108438    -2.156089     2.119531
H     75    -4.012074     1.974322     3.871778
H     76     4.012074    -1.974322     3.871778
S     77     4.519698     6.839899     0.277494
C     78     4.510947     8.301905    -0.646682
C     79     3.518090     8.295015    -1.588057
```

```
C      80      2.730980      7.097626     -1.598450
H      81      5.237058      9.077091     -0.441933
H      82      3.350187      9.115432     -2.277815
C      83      1.611644      6.896078     -2.591434
C      84      0.301387      7.617681     -2.210096
C      85     -0.802961      7.433869     -3.258744
C      86     -2.110583      8.152139     -2.900205
C      87     -3.217521      7.971120     -3.947645
C      88     -4.519698      8.694021     -3.583663
H      89      1.946799      7.274682     -3.565749
H      90      1.411196      5.828280     -2.727879
H      91      0.505683      8.688240     -2.075720
H      92     -0.049015      7.247093     -1.237625
H      93     -0.442514      7.800717     -4.230704
H      94     -1.002574      6.360726     -3.390970
H      95     -1.910367      9.225557     -2.768783
H      96     -2.471071      7.786367     -1.927767
H      97     -2.857026      8.335188     -4.919765
H      98     -3.418934      6.898767     -4.077822
H      99     -4.356857      9.773611     -3.480373
H     100     -4.922763      8.327142     -2.632055
H     101     -5.287731      8.544683     -4.350530
S     102     -4.519698     -6.839899      0.277494
C     103     -4.510947     -8.301905     -0.646682
C     104     -3.518090     -8.295015     -1.588057
C     105     -2.730980     -7.097626     -1.598450
H     106     -5.237058     -9.077091     -0.441933
H     107     -3.350187     -9.115432     -2.277815
C     108     -1.611644     -6.896078     -2.591434
C     109     -0.301387     -7.617681     -2.210096
C     110      0.802961     -7.433869     -3.258744
C     111      2.110583     -8.152139     -2.900205
C     112      3.217521     -7.971120     -3.947645
C     113      4.519698     -8.694021     -3.583663
H     114     -1.411196     -5.828280     -2.727879
H     115     -1.946799     -7.274682     -3.565749
H     116      0.049015     -7.247093     -1.237625
H     117     -0.505683     -8.688240     -2.075720
H     118      1.002574     -6.360726     -3.390970
H     119      0.442514     -7.800717     -4.230704
H     120      2.471071     -7.786367     -1.927767
H     121      1.910367     -9.225557     -2.768783
H     122      3.418934     -6.898767     -4.077822
H     123      2.857026     -8.335188     -4.919765
H     124      4.922763     -8.327142     -2.632055
H     125      4.356857     -9.773611     -3.480373
H     126      5.287731     -8.544683     -4.350530


T3-B
C       1      0.428836      0.566142     -0.157406
C       2     -0.428836     -0.566142     -0.157406
```

```
C     3      1.791393     0.094695    -0.175371
C     4     -1.791393    -0.094695    -0.175371
C     5      0.344719    -1.737251    -0.185416
C     6     -0.344719     1.737251    -0.185416
N     7      1.680721    -1.328085    -0.194804
N     8     -1.680721     1.328085    -0.194804
O     9      2.885472     0.675848    -0.171562
O    10     -2.885472    -0.675848    -0.171562
C    11     -0.142848    -3.087129    -0.222454
C    12      0.142848     3.087129    -0.222454
S    13      0.843960    -4.543342    -0.365144
S    14     -0.843960     4.543342    -0.365144
C    15     -0.563675    -5.584476    -0.348871
C    16      0.563675     5.584476    -0.348871
C    17     -1.722203    -4.825693    -0.235699
C    18      1.722203     4.825693    -0.235699
C    19     -1.491297    -3.441207    -0.167530
C    20      1.491297     3.441207    -0.167530
C    21     -0.425761    -7.015331    -0.445435
C    22      0.425761     7.015331    -0.445435
H    23     -2.713733    -5.263048    -0.208537
H    24      2.713733     5.263048    -0.208537
H    25     -2.274494    -2.695101    -0.089217
H    26      2.274494     2.695101    -0.089217
C    27      2.898887    -2.137089    -0.123759
C    28     -2.898887     2.137089    -0.123759
C    29      3.281430    -2.548964     1.305304
C    30     -3.281430     2.548964     1.305304
C    31      4.578032    -3.368089     1.338892
C    32     -4.578032     3.368089     1.338892
C    33      5.000147    -3.772689     2.757727
C    34     -5.000147     3.772689     2.757727
C    35      6.297026    -4.591752     2.799268
C    36     -6.297026     4.591752     2.799268
C    37      6.721886    -4.996601     4.216983
C    38     -6.721886     4.996601     4.216983
C    39      8.018883    -5.815567     4.260897
C    40     -8.018883     5.815567     4.260897
C    41      8.435563    -6.216007     5.681050
C    42     -8.435563     6.216007     5.681050
H    43      3.688419    -1.512414    -0.548248
H    44     -3.688419     1.512414    -0.548248
H    45      2.795429    -3.005627    -0.778034
H    46     -2.795429     3.005627    -0.778034
H    47      3.398938    -1.640714     1.909199
H    48     -3.398938     1.640714     1.909199
H    49      2.466567    -3.127849     1.757048
H    50     -2.466567     3.127849     1.757048
H    51      5.386367    -2.787563     0.871974
H    52     -5.386367     2.787563     0.871974
H    53      4.453947    -4.272480     0.726070
```

```
H     54    -4.453947     4.272480     0.726070
H     55     5.123457    -2.867516     3.369417
H     56    -5.123457     2.867516     3.369417
H     57     4.190491    -4.351572     3.224868
H     58    -4.190491     4.351572     3.224868
H     59     7.105881    -4.012315     2.330839
H     60    -7.105881     4.012315     2.330839
H     61     6.173399    -5.496649     2.186513
H     62    -6.173399     5.496649     2.186513
H     63     6.845718    -4.092128     4.830494
H     64    -6.845718     4.092128     4.830494
H     65     5.913408    -5.576318     4.686205
H     66    -5.913408     5.576318     4.686205
H     67     8.827064    -5.236402     3.792862
H     68    -8.827064     5.236402     3.792862
H     69     7.895652    -6.719401     3.648025
H     70    -7.895652     6.719401     3.648025
H     71     8.599473    -5.331858     6.308845
H     72    -8.599473     5.331858     6.308845
H     73     7.661500    -6.825373     6.162961
H     74    -7.661500     6.825373     6.162961
H     75     9.363591    -6.798371     5.676874
H     76    -9.363591     6.798371     5.676874
S     77    -1.831154    -8.066521    -0.314591
C     78     0.717500    -7.772165    -0.641081
C     79     0.477634    -9.164671    -0.697170
C     80    -0.855270    -9.507932    -0.545031
H     81     1.260294    -9.896864    -0.859701
H     82     1.703588    -7.335748    -0.754702
S     83    -0.477634   -12.275542    -0.479068
C     84    -1.884224   -13.318226    -0.532323
C     85    -3.031872   -12.564484    -0.594215
C     86    -2.801305   -11.159920    -0.606673
C     87    -1.463872   -10.820051    -0.552064
H     88    -3.596788   -10.424858    -0.664574
H     89    -4.020203   -13.010103    -0.632700
C     90    -1.749035   -14.814608    -0.530666
C     91    -1.181225   -15.403596    -1.839626
C     92    -1.097816   -16.934819    -1.812234
C     93    -0.536608   -17.535845    -3.107697
C     94    -0.449616   -19.067811    -3.086450
C     95     0.111917   -19.660181    -4.384315
H     96    -1.117420   -15.134431     0.308743
H     97    -2.745888   -15.233329    -0.347474
H     98    -0.182394   -14.985963    -2.022606
H     99    -1.812193   -15.081062    -2.678247
H    100    -0.470809   -17.248645    -0.965170
H    101    -2.098810   -17.349213    -1.624230
H    102     0.463986   -17.120335    -3.296531
H    103    -1.163835   -17.221701    -3.954654
H    104     0.177318   -19.381775    -2.240338
```

```
H    105    -1.449237    -19.483313    -2.897706
H    106     1.124734    -19.289186    -4.582310
H    107    -0.513325    -19.391528    -5.244279
H    108     0.160920    -20.753616    -4.336536
S    109     1.831154      8.066521    -0.314591
C    110    -0.717500      7.772165    -0.641081
C    111    -0.477634      9.164671    -0.697170
C    112     0.855270      9.507932    -0.545031
H    113    -1.260294      9.896864    -0.859701
H    114    -1.703588      7.335748    -0.754702
S    115     0.477634     12.275542    -0.479068
C    116     1.884224     13.318226    -0.532323
C    117     3.031872     12.564484    -0.594215
C    118     2.801305     11.159920    -0.606673
C    119     1.463872     10.820051    -0.552064
H    120     3.596788     10.424858    -0.664574
H    121     4.020203     13.010103    -0.632700
C    122     1.749035     14.814608    -0.530666
C    123     1.181225     15.403596    -1.839626
C    124     1.097816     16.934819    -1.812234
C    125     0.536608     17.535845    -3.107697
C    126     0.449616     19.067811    -3.086450
C    127    -0.111917     19.660181    -4.384315
H    128     1.117420     15.134431     0.308743
H    129     2.745888     15.233329    -0.347474
H    130     0.182394     14.985963    -2.022606
H    131     1.812193     15.081062    -2.678247
H    132     0.470809     17.248645    -0.965170
H    133     2.098810     17.349213    -1.624230
H    134    -0.463986     17.120335    -3.296531
H    135     1.163835     17.221701    -3.954654
H    136    -0.177318     19.381775    -2.240338
H    137     1.449237     19.483313    -2.897706
H    138    -1.124734     19.289186    -4.582310
H    139     0.513325     19.391528    -5.244279
H    140    -0.160920     20.753616    -4.336536

T3-A
C      1     0.418260      0.574111     0.361947
C      2    -0.418260     -0.574111     0.361947
C      3     1.791081      0.130251     0.305137
C      4    -1.791081     -0.130251     0.305137
C      5     0.375939     -1.725009     0.278975
C      6    -0.375939      1.725009     0.278975
N      7     1.707613     -1.295887     0.278167
N      8    -1.707613      1.295887     0.278167
O      9     2.867802      0.739374     0.295167
O     10    -2.867802     -0.739374     0.295167
C     11    -0.087007     -3.078662     0.151106
C     12     0.087007      3.078662     0.151106
S     13     0.893420     -4.452621    -0.359856
```

```
S    14   -0.893420    4.452621   -0.359856
C    15   -0.474450   -5.544133   -0.286855
C    16    0.474450    5.544133   -0.286855
C    17   -1.617984   -4.857977    0.102838
C    18    1.617984    4.857977    0.102838
C    19   -1.406089   -3.488216    0.339136
C    20    1.406089    3.488216    0.339136
C    21   -0.323730   -6.940138   -0.610612
C    22    0.323730    6.940138   -0.610612
H    23   -2.583003   -5.337614    0.220126
H    24    2.583003    5.337614    0.220126
H    25   -2.185948   -2.792040    0.624442
H    26    2.185948    2.792040    0.624442
C    27    2.925818   -2.100884    0.405824
C    28   -2.925818    2.100884    0.405824
C    29    3.131873   -2.753032    1.793930
C    30   -3.131873    2.753032    1.793930
C    31    4.318574   -3.735428    1.702104
C    32   -4.318574    3.735428    1.702104
C    33    4.565512   -4.568915    2.967388
C    34   -4.565512    4.568915    2.967388
C    35    5.677133   -5.612829    2.791417
C    36   -5.677133    5.612829    2.791417
C    37    5.932230   -6.443144    4.054792
C    38   -5.932230    6.443144    4.054792
C    39    3.257317   -1.717352    2.935592
C    40   -3.257317    1.717352    2.935592
C    41    4.541918   -0.876668    2.952290
C    42   -4.541918    0.876668    2.952290
H    43    3.744482   -1.413233    0.182298
H    44   -3.744482    1.413233    0.182298
H    45    2.936763   -2.864423   -0.376682
H    46   -2.936763    2.864423   -0.376682
H    47    6.728494   -7.178590    3.895652
H    48   -6.728494    7.178590    3.895652
H    49    2.236380   -3.350506    2.012017
H    50   -2.236380    3.350506    2.012017
H    51    5.235082   -3.187740    1.442276
H    52   -5.235082    3.187740    1.442276
H    53    4.131563   -4.422780    0.865238
H    54   -4.131563    4.422780    0.865238
H    55    4.826526   -3.911949    3.807410
H    56   -4.826526    3.911949    3.807410
H    57    3.633681   -5.078424    3.253273
H    58   -3.633681    5.078424    3.253273
H    59    6.605304   -5.104837    2.494737
H    60   -6.605304    5.104837    2.494737
H    61    5.415636   -6.282646    1.960512
H    62   -5.415636    6.282646    1.960512
H    63    6.231329   -5.804020    4.894220
H    64   -6.231329    5.804020    4.894220
```

```
H      65      5.030322     -6.988224      4.358233
H      66     -5.030322      6.988224      4.358233
H      67      3.167296     -2.250568      3.889603
H      68     -3.167296      2.250568      3.889603
H      69      2.389307     -1.047368      2.893347
H      70     -2.389307      1.047368      2.893347
H      71      5.434255     -1.496865      3.088789
H      72     -5.434255      1.496865      3.088789
H      73      4.662638     -0.302179      2.028939
H      74     -4.662638      0.302179      2.028939
H      75      4.512043     -0.160949      3.781171
H      76     -4.512043      0.160949      3.781171
S      77     -1.723299     -8.004570     -0.683056
C      78      0.829059     -7.649799     -0.902431
C      79      0.603957     -9.020722     -1.166911
C      80     -0.727125     -9.393570     -1.085142
H      81      1.399400     -9.720367     -1.396959
H      82      1.814691     -7.198080     -0.913533
S      83     -0.388257    -12.019905     -1.975470
C      84     -1.743615    -13.124795     -1.873740
C      85     -2.838794    -12.485190     -1.344061
C      86     -2.606492    -11.120906     -1.010721
C      87     -1.321196    -10.697085     -1.285635
H      88     -3.361266    -10.476492     -0.573148
H      89     -3.790028    -12.985023     -1.195069
C      90     -1.617984    -14.557513     -2.308393
C      91     -0.752320    -15.431935     -1.376267
C      92     -0.685842    -16.895206     -1.831089
C      93      0.171585    -17.778039     -0.914652
C      94      0.241699    -19.243587     -1.364333
C      95      1.100654    -20.118662     -0.443955
H      96     -2.630854    -14.974766     -2.358940
H      97     -1.209092    -14.607086     -3.326314
H      98     -1.159270    -15.377823     -0.357977
H      99      0.263163    -15.017070     -1.328492
H     100     -1.704556    -17.306095     -1.880703
H     101     -0.286225    -16.939003     -2.854581
H     102     -0.227610    -17.733407      0.109116
H     103      1.190398    -17.366930     -0.864655
H     104     -0.776142    -19.654745     -1.413969
H     105      0.640305    -19.288309     -2.387389
H     106      0.706922    -20.121031      0.579576
H     107      2.133317    -19.752073     -0.400842
H     108      1.129873    -21.157014     -0.792181
S     109      1.723299      8.004570     -0.683056
C     110     -0.829059      7.649799     -0.902431
C     111     -0.603957      9.020722     -1.166911
C     112      0.727125      9.393570     -1.085142
H     113     -1.399400      9.720367     -1.396959
H     114     -1.814691      7.198080     -0.913533
S     115      0.388257     12.019905     -1.975470
```

```
C    116    1.743615    13.124795    -1.873740
C    117    2.838794    12.485190    -1.344061
C    118    2.606492    11.120906    -1.010721
C    119    1.321196    10.697085    -1.285635
H    120    3.361266    10.476492    -0.573148
H    121    3.790028    12.985023    -1.195069
C    122    1.617984    14.557513    -2.308393
C    123    0.752320    15.431935    -1.376267
C    124    0.685842    16.895206    -1.831089
C    125   -0.171585    17.778039    -0.914652
C    126   -0.241699    19.243587    -1.364333
C    127   -1.100654    20.118662    -0.443955
H    128    1.209092    14.607086    -3.326314
H    129    2.630854    14.974766    -2.358940
H    130   -0.263163    15.017070    -1.328492
H    131    1.159270    15.377823    -0.357977
H    132    0.286225    16.939003    -2.854581
H    133    1.704556    17.306095    -1.880703
H    134   -1.190398    17.366930    -0.864655
H    135    0.227610    17.733407     0.109116
H    136   -0.640305    19.288309    -2.387389
H    137    0.776142    19.654745    -1.413969
H    138   -2.133317    19.752073    -0.400842
H    139   -0.706922    20.121031     0.579576
H    140   -1.129873    21.157014    -0.792181
```

c) Cation-radical in dichloromethane calculated by PCM/B3LYP/6-31++G(d,p) method

T1-B
```
C      1   -0.691399     0.018804    -1.278361
C      2    0.691399    -0.018804    -1.278361
C      3   -1.104442     1.417546    -1.283852
C      4    1.104442    -1.417546    -1.283852
C      5    1.214001     1.323356    -1.281955
C      6   -1.214001    -1.323356    -1.281955
N      7    0.125292     2.158099    -1.288008
N      8   -0.125292    -2.158099    -1.288008
O      9   -2.199393     1.960460    -1.291543
O     10    2.199393    -1.960460    -1.291543
C     11    2.587129     1.686578    -1.286094
C     12   -2.587129    -1.686578    -1.286094
S     13    3.226258     3.332449    -1.251002
S     14   -3.226258    -3.332449    -1.251002
C     15    4.839428     2.752056    -1.275640
C     16   -4.839428    -2.752056    -1.275640
C     17    4.914157     1.372379    -1.309898
C     18   -4.914157    -1.372379    -1.309898
C     19    3.648311     0.766075    -1.314096
C     20   -3.648311    -0.766075    -1.314096
H     21    5.657072     3.461344    -1.264326
H     22   -5.657072    -3.461344    -1.264326
```

```
H   23    5.849295    0.827099   -1.329027
H   24   -5.849295   -0.827099   -1.329027
H   25    3.485961   -0.304890   -1.335472
H   26   -3.485961    0.304890   -1.335472
C   27    0.066179    3.628200   -1.284898
C   28   -0.066179   -3.628200   -1.284898
C   29    0.093634    4.234840    0.124819
C   30   -0.093634   -4.234840    0.124819
C   31    0.003811    5.766026    0.081626
C   32   -0.003811   -5.766026    0.081626
C   33   -0.003811    6.405467    1.476693
C   34    0.003811   -6.405467    1.476693
C   35   -0.094695    7.936768    1.441638
C   36    0.094695   -7.936768    1.441638
C   37   -0.103695    8.582229    2.833575
C   38    0.103695   -8.582229    2.833575
C   39   -0.195076   10.113665    2.800083
C   40    0.195076  -10.113665    2.800083
C   41   -0.203027   10.751107    4.194421
C   42    0.203027  -10.751107    4.194421
H   43   -0.873553    3.881965   -1.779841
H   44    0.873553   -3.881965   -1.779841
H   45    0.871335    4.011524   -1.914579
H   46   -0.871335   -4.011524   -1.914579
H   47   -0.749470    3.827956    0.695632
H   48    0.749470   -3.827956    0.695632
H   49    1.008592    3.931538    0.647367
H   50   -1.008592   -3.931538    0.647367
H   51   -0.907072    6.060838   -0.457674
H   52    0.907072   -6.060838   -0.457674
H   53    0.849127    6.165471   -0.496076
H   54   -0.849127   -6.165471   -0.496076
H   55   -0.849580    6.004676    2.053190
H   56    0.849580   -6.004676    2.053190
H   57    0.906354    6.107948    2.016800
H   58   -0.906354   -6.107948    2.016800
H   59   -1.004624    8.232530    0.899723
H   60    1.004624   -8.232530    0.899723
H   61    0.750764    8.336309    0.862971
H   62   -0.750764   -8.336309    0.862971
H   63   -0.949055    8.183105    3.413010
H   64    0.949055   -8.183105    3.413010
H   65    0.806296    8.287052    3.376360
H   66   -0.806296   -8.287052    3.376360
H   67   -1.104468   10.408802    2.258406
H   68    1.104468  -10.408802    2.258406
H   69    0.649243   10.512721    2.220874
H   70   -0.649243  -10.512721    2.220874
H   71   -1.055812   10.396957    4.786009
H   72    1.055812  -10.396957    4.786009
H   73    0.710400   10.502355    4.748010
```

```
H     74    -0.710400   -10.502355    4.748010
H     75    -0.269476    11.842987    4.134700
H     76     0.269476   -11.842987    4.134700


T1-A
C      1    -0.688715     0.061894   -0.877410
C      2     0.688715    -0.061894   -0.877410
C      3    -1.014464     1.483589   -0.909213
C      4     1.014464    -1.483589   -0.909213
C      5     1.292897     1.244118   -0.916339
C      6    -1.292897    -1.244118   -0.916339
N      7     0.259147     2.148467   -0.900344
N      8    -0.259147    -2.148467   -0.900344
O      9    -2.076072     2.087164   -0.941083
O     10     2.076072    -2.087164   -0.941083
C     11     2.684672     1.517760   -0.998157
C     12    -2.684672    -1.517760   -0.998157
S     13     3.417496     3.105834   -1.238291
S     14    -3.417496    -3.105834   -1.238291
C     15     4.991898     2.426612   -1.243422
C     16    -4.991898    -2.426612   -1.243422
C     17     4.986237     1.055497   -1.068871
C     18    -4.986237    -1.055497   -1.068871
C     19     3.688825     0.536955   -0.935137
C     20    -3.688825    -0.536955   -0.935137
H     21     5.847674     3.075251   -1.379830
H     22    -5.847674    -3.075251   -1.379830
H     23     5.886570     0.454805   -1.041858
H     24    -5.886570    -0.454805   -1.041858
H     25     3.464368    -0.514644   -0.804670
H     26    -3.464368     0.514644   -0.804670
C     27     0.309259     3.618920   -0.828618
C     28    -0.309259    -3.618920   -0.828618
C     29     0.653680     4.182174    0.571120
C     30    -0.653680    -4.182174    0.571120
C     31     0.911561     5.697949    0.431438
C     32    -0.911561    -5.697949    0.431438
C     33     1.394981     6.385201    1.716395
C     34    -1.394981    -6.385201    1.716395
C     35     1.763562     7.860019    1.502722
C     36    -1.763562    -7.860019    1.502722
C     37     2.237869     8.554464    2.784480
C     38    -2.237869    -8.554464    2.784480
C     39    -0.396526     3.816939    1.646721
C     40     0.396526    -3.816939    1.646721
C     41    -1.763562     4.504545    1.525539
C     42     1.763562    -4.504545    1.525539
H     43    -0.680327     3.953713   -1.144848
H     44     0.680327    -3.953713   -1.144848
H     45     1.015534     3.976672   -1.581300
H     46    -1.015534    -3.976672   -1.581300
```

```
H    47    2.494807    9.602829    2.598111
H    48   -2.494807   -9.602829    2.598111
H    49    1.598449    3.723094    0.891369
H    50   -1.598449   -3.723094    0.891369
H    51    0.002840    6.197740    0.069688
H    52   -0.002840   -6.197740    0.069688
H    53    1.669770    5.849493   -0.349147
H    54   -1.669770   -5.849493   -0.349147
H    55    0.621567    6.322154    2.492726
H    56   -0.621567   -6.322154    2.492726
H    57    2.270260    5.847169    2.108627
H    58   -2.270260   -5.847169    2.108627
H    59    0.892910    8.394438    1.098328
H    60   -0.892910   -8.394438    1.098328
H    61    2.548633    7.929191    0.737147
H    62   -2.548633   -7.929191    0.737147
H    63    1.459618    8.533915    3.556637
H    64   -1.459618   -8.533915    3.556637
H    65    3.126644    8.061158    3.195899
H    66   -3.126644   -8.061158    3.195899
H    67    0.034072    4.050767    2.627062
H    68   -0.034072   -4.050767    2.627062
H    69   -0.536520    2.728267    1.646990
H    70    0.536520   -2.728267    1.646990
H    71   -1.682452    5.591707    1.625325
H    72    1.682452   -5.591707    1.625325
H    73   -2.250443    4.286142    0.570323
H    74    2.250443   -4.286142    0.570323
H    75   -2.430649    4.152825    2.319658
H    76    2.430649   -4.152825    2.319658

T2-B
C     1   -0.387714   -0.575783   -0.341015
C     2    0.387714    0.575783   -0.341015
C     3   -1.789641   -0.177623   -0.347703
C     4    1.789641    0.177623   -0.347703
C     5   -0.463192    1.730263   -0.346435
C     6    0.463192   -1.730263   -0.346435
N     7   -1.761404    1.246859   -0.353886
N     8    1.761404   -1.246859   -0.353886
O     9   -2.835142   -0.822130   -0.352059
O    10    2.835142    0.822130   -0.352059
C    11   -0.043552    3.078011   -0.352056
C    12    0.043552   -3.078011   -0.352056
S    13   -1.095396    4.498224   -0.359986
S    14    1.095396   -4.498224   -0.359986
C    15    0.271876    5.586917   -0.358886
C    16   -0.271876   -5.586917   -0.358886
C    17    1.476964    4.867486   -0.353088
C    18   -1.476964   -4.867486   -0.353088
C    19    1.306406    3.489603   -0.349411
```

```
C    20    -1.306406    -3.489603    -0.349411
C    21     0.091497     7.003756    -0.366394
C    22    -0.091497    -7.003756    -0.366394
H    23     2.447278     5.349076    -0.350746
H    24    -2.447278    -5.349076    -0.350746
H    25     2.122149     2.775554    -0.345013
H    26    -2.122149    -2.775554    -0.345013
C    27    -3.031530     1.983816    -0.324815
C    28     3.031530    -1.983816    -0.324815
C    29    -3.501311     2.332526     1.094225
C    30     3.501311    -2.332526     1.094225
C    31    -4.847943     3.067654     1.084102
C    32     4.847943    -3.067654     1.084102
C    33    -5.356815     3.406069     2.491806
C    34     5.356815    -3.406069     2.491806
C    35    -6.706105     4.136633     2.493507
C    36     6.706105    -4.136633     2.493507
C    37    -7.217658     4.474125     3.900192
C    38     7.217658    -4.474125     3.900192
C    39    -8.567854     5.203277     3.905690
C    40     8.567854    -5.203277     3.905690
C    41    -9.070878     5.536847     5.315074
C    42     9.070878    -5.536847     5.315074
H    43    -3.760906     1.327670    -0.804840
H    44     3.760906    -1.327670    -0.804840
H    45    -2.939952     2.870346    -0.955758
H    46     2.939952    -2.870346    -0.955758
H    47    -3.589329     1.402940     1.669380
H    48     3.589329    -1.402940     1.669380
H    49    -2.746537     2.948352     1.598133
H    50     2.746537    -2.948352     1.598133
H    51    -5.594772     2.448963     0.567205
H    52     5.594772    -2.448963     0.567205
H    53    -4.754812     3.993532     0.498880
H    54     4.754812    -3.993532     0.498880
H    55    -5.446013     2.478822     3.075501
H    56     5.446013    -2.478822     3.075501
H    57    -4.608723     4.024288     3.008447
H    58     4.608723    -4.024288     3.008447
H    59    -7.453051     3.517734     1.975630
H    60     7.453051    -3.517734     1.975630
H    61    -6.616964     5.063700     1.908632
H    62     6.616964    -5.063700     1.908632
H    63    -7.306122     3.547243     4.485658
H    64     7.306122    -3.547243     4.485658
H    65    -6.471198     5.093648     4.418706
H    66     6.471198    -5.093648     4.418706
H    67    -9.314100     4.584133     3.388676
H    68     9.314100    -4.584133     3.388676
H    69    -8.480161     6.129339     3.320539
H    70     8.480161    -6.129339     3.320539
```

```
H      71     -9.200974      4.627329      5.913818
H      72      9.200974     -4.627329      5.913818
H      73     -8.361549      6.183768      5.845218
H      74      8.361549     -6.183768      5.845218
H      75    -10.035339      6.055532      5.283356
H      76     10.035339     -6.055532      5.283356
S      77      1.468918      8.101151     -0.362077
C      78      0.433639      9.501074     -0.368456
C      79     -0.898504      9.126359     -0.373412
C      80     -1.095396      7.729811     -0.372911
H      81     -2.074109      7.263127     -0.375613
H      82     -1.706097      9.849593     -0.375127
C      83      0.998363     10.890418     -0.401229
C      84      1.573117     11.298183     -1.777215
C      85      2.096568     12.739682     -1.789248
C      86      2.667400     13.163338     -3.149113
C      87      3.192568     14.605155     -3.170081
C      88      3.760731     15.021729     -4.531741
H      89      0.193664     11.580821     -0.124315
H      90      1.781325     10.994140      0.360277
H      91      0.791778     11.180062     -2.538882
H      92      2.383658     10.609858     -2.049428
H      93      1.282845     13.423328     -1.508308
H      94      2.872677     12.850201     -1.018539
H      95      1.890780     13.050799     -3.919479
H      96      3.480748     12.478803     -3.430524
H      97      2.380060     15.289132     -2.888396
H      98      3.968613     14.717612     -2.400364
H      99      2.997820     14.952174     -5.316404
H     100      4.597757     14.376754     -4.824935
H     101      4.126292     16.054252     -4.513028
S     102     -1.468918     -8.101151     -0.362077
C     103     -0.433639     -9.501074     -0.368456
C     104      0.898504     -9.126359     -0.373412
C     105      1.095396     -7.729811     -0.372911
H     106      2.074109     -7.263127     -0.375613
H     107      1.706097     -9.849593     -0.375127
C     108     -0.998363    -10.890418     -0.401229
C     109     -1.573117    -11.298183     -1.777215
C     110     -2.096568    -12.739682     -1.789248
C     111     -2.667400    -13.163338     -3.149113
C     112     -3.192568    -14.605155     -3.170081
C     113     -3.760731    -15.021729     -4.531741
H     114     -1.781325    -10.994140      0.360277
H     115     -0.193664    -11.580821     -0.124315
H     116     -2.383658    -10.609858     -2.049428
H     117     -0.791778    -11.180062     -2.538882
H     118     -2.872677    -12.850201     -1.018539
H     119     -1.282845    -13.423328     -1.508308
H     120     -3.480748    -12.478803     -3.430524
H     121     -1.890780    -13.050799     -3.919479
```

```
H   122   -3.968613   -14.717612   -2.400364
H   123   -2.380060   -15.289132   -2.888396
H   124   -4.597757   -14.376754   -4.824935
H   125   -2.997820   -14.952174   -5.316404
H   126   -4.126292   -16.054252   -4.513028
```

T2-A
```
C     1   -0.647894   -0.248730   -0.526606
C     2    0.647894    0.248730   -0.526606
C     3   -1.568257    0.881716   -0.555538
C     4    1.568257   -0.881716   -0.555538
C     5    0.613340    1.680645   -0.575353
C     6   -0.613340   -1.680645   -0.575353
N     7   -0.728016    2.034122   -0.553175
N     8    0.728016   -2.034122   -0.553175
O     9   -2.793875    0.946733   -0.574785
O    10    2.793875   -0.946733   -0.574785
C    11    1.728900    2.538767   -0.688491
C    12   -1.728900   -2.538767   -0.688491
S    13    1.673805    4.283085   -0.961647
S    14   -1.673805   -4.283085   -0.961647
C    15    3.417356    4.394367   -1.004610
C    16   -3.417356   -4.394367   -1.004610
C    17    3.998081    3.130712   -0.813374
C    18   -3.998081   -3.130712   -0.813374
C    19    3.072621    2.109311   -0.645391
C    20   -3.072621   -2.109311   -0.645391
C    21    4.074655    5.644295   -1.219183
C    22   -4.074655   -5.644295   -1.219183
H    23    5.069726    2.972761   -0.800239
H    24   -5.069726   -2.972761   -0.800239
H    25    3.335782    1.067818   -0.501363
H    26   -3.335782   -1.067818   -0.501363
C    27   -1.327848    3.372506   -0.449741
C    28    1.327848   -3.372506   -0.449741
C    29   -1.225475    4.018877    0.952534
C    30    1.225475   -4.018877    0.952534
C    31   -1.673805    5.491820    0.841532
C    32    1.673805   -5.491820    0.841532
C    33   -1.498250    6.314362    2.125795
C    34    1.498250   -6.314362    2.125795
C    35   -1.841579    7.798748    1.938021
C    36    1.841579   -7.798748    1.938021
C    37   -1.673805    8.623604    3.219327
C    38    1.673805   -8.623604    3.219327
C    39   -1.967729    3.214589    2.045725
C    40    1.967729   -3.214589    2.045725
C    41   -3.501145    3.222041    1.972822
C    42    3.501145   -3.222041    1.972822
H    43   -2.373279    3.239144   -0.734491
H    44    2.373279   -3.239144   -0.734491
```

```
H    45    -0.878452     4.017870    -1.208508
H    46     0.878452    -4.017870    -1.208508
H    47    -1.924875     9.676598     3.051678
H    48     1.924875    -9.676598     3.051678
H    49    -0.164806     4.025548     1.237791
H    50     0.164806    -4.025548     1.237791
H    51    -2.723182     5.536899     0.519795
H    52     2.723182    -5.536899     0.519795
H    53    -1.092925     5.970526     0.040880
H    54     1.092925    -5.970526     0.040880
H    55    -2.127370     5.903938     2.926191
H    56     2.127370    -5.903938     2.926191
H    57    -0.459012     6.225056     2.474402
H    58     0.459012    -6.225056     2.474402
H    59    -2.876495     7.886990     1.579683
H    60     2.876495    -7.886990     1.579683
H    61    -1.206278     8.219574     1.146362
H    62     1.206278    -8.219574     1.146362
H    63    -2.324104     8.248902     4.018729
H    64     2.324104    -8.248902     4.018729
H    65    -0.640749     8.580890     3.584784
H    66     0.640749    -8.580890     3.584784
H    67    -1.655433     3.605017     3.021282
H    68     1.655433    -3.605017     3.021282
H    69    -1.609435     2.177470     2.021889
H    70     1.609435    -2.177470     2.021889
H    71    -3.910265     4.229852     2.098119
H    72     3.910265    -4.229852     2.098119
H    73    -3.867534     2.821076     1.022986
H    74     3.867534    -2.821076     1.022986
H    75    -3.917044     2.599407     2.772172
H    76     3.917044    -2.599407     2.772172
S    77     5.830542     5.751486    -1.302068
C    78     5.776405     7.471000    -1.568347
C    79     4.468614     7.922890    -1.591838
C    80     3.512309     6.904755    -1.397018
H    81     2.442729     7.082928    -1.387780
H    82     4.216386     8.965462    -1.748693
C    83     7.031918     8.280197    -1.706649
C    84     7.785396     8.497708    -0.374402
C    85     9.032336     9.374296    -0.544022
C    86     9.792490     9.603769     0.769028
C    87    11.040639    10.481944     0.608036
C    88    11.795103    10.707041     1.923555
H    89     7.707175     7.802490    -2.427415
H    90     6.753431     9.252052    -2.129570
H    91     8.073803     7.523862     0.041994
H    92     7.102320     8.959260     0.350126
H    93     9.705938     8.908976    -1.277711
H    94     8.738026    10.345168    -0.967367
H    95    10.086620     8.632541     1.192673
```

```
H    96     9.117279    10.067250     1.502884
H    97    11.715207    10.019189    -0.125561
H    98    10.746652    11.452340     0.184670
H    99    12.131349     9.756191     2.354118
H   100    11.156333    11.199912     2.666264
H   101    12.679221    11.336433     1.774284
S   102    -5.830542    -5.751486    -1.302068
C   103    -5.776405    -7.471000    -1.568347
C   104    -4.468614    -7.922890    -1.591838
C   105    -3.512309    -6.904755    -1.397018
H   106    -2.442729    -7.082928    -1.387780
H   107    -4.216386    -8.965462    -1.748693
C   108    -7.031918    -8.280197    -1.706649
C   109    -7.785396    -8.497708    -0.374402
C   110    -9.032336    -9.374296    -0.544022
C   111    -9.792490    -9.603769     0.769028
C   112   -11.040639   -10.481944     0.608036
C   113   -11.795103   -10.707041     1.923555
H   114    -6.753431    -9.252052    -2.129570
H   115    -7.707175    -7.802490    -2.427415
H   116    -7.102320    -8.959260     0.350126
H   117    -8.073803    -7.523862     0.041994
H   118    -8.738026   -10.345168    -0.967367
H   119    -9.705938    -8.908976    -1.277711
H   120    -9.117279   -10.067250     1.502884
H   121   -10.086620    -8.632541     1.192673
H   122   -10.746652   -11.452340     0.184670
H   123   -11.715207   -10.019189    -0.125561
H   124   -11.156333   -11.199912     2.666264
H   125   -12.131349    -9.756191     2.354118
H   126   -12.679221   -11.336433     1.774284
```

T2-D

```
C     1    -0.670000    -0.180718     0.648711
C     2     0.670000     0.180718     0.648711
C     3    -1.467834     1.039165     0.671330
C     4     1.467834    -1.039165     0.671330
C     5     0.783998     1.610093     0.689171
C     6    -0.783998    -1.610093     0.689171
N     7    -0.511380     2.097336     0.698740
N     8     0.511380    -2.097336     0.698740
O     9    -2.678887     1.237164     0.658140
O    10     2.678887    -1.237164     0.658140
C    11     1.985685     2.350628     0.738396
C    12    -1.985685    -2.350628     0.738396
S    13     2.127392     4.097316     0.956952
S    14    -2.127392    -4.097316     0.956952
C    15     3.873805     4.028408     0.934142
C    16    -3.873805    -4.028408     0.934142
C    17     4.304248     2.704708     0.738905
C    18    -4.304248    -2.704708     0.738905
```

```
C    19     3.272423     1.781907     0.643039
C    20    -3.272423    -1.781907     0.643039
C    21     4.714626     5.184075     1.072969
C    22    -4.714626    -5.184075     1.072969
H    23     5.351314     2.430816     0.699675
H    24    -5.351314    -2.430816     0.699675
H    25     3.421081     0.714816     0.525243
H    26    -3.421081    -0.714816     0.525243
C    27    -0.984359     3.481718     0.557902
C    28     0.984359    -3.481718     0.557902
C    29    -1.007414     3.954960    -0.902371
C    30     1.007414    -3.954960    -0.902371
C    31    -1.599289     5.362734    -1.047782
C    32     1.599289    -5.362734    -1.047782
C    33    -1.670288     5.827910    -2.508874
C    34     1.670288    -5.827910    -2.508874
C    35    -2.276199     7.227215    -2.678580
C    36     2.276199    -7.227215    -2.678580
C    37    -2.351644     7.686356    -4.140841
C    38     2.351644    -7.686356    -4.140841
C    39    -2.954594     9.086453    -4.316910
C    40     2.954594    -9.086453    -4.316910
C    41    -3.029743     9.533787    -5.781502
C    42     3.029743    -9.533787    -5.781502
H    43    -0.383022     4.133887     1.193714
H    44     0.383022    -4.133887     1.193714
H    45    -1.996390     3.485559     0.967862
H    46     1.996390    -3.485559     0.967862
H    47     0.007805     3.934666    -1.317481
H    48    -0.007805    -3.934666    -1.317481
H    49    -1.603834     3.243135    -1.486100
H    50     1.603834    -3.243135    -1.486100
H    51    -0.998752     6.076368    -0.466737
H    52     0.998752    -6.076368    -0.466737
H    53    -2.608019     5.378821    -0.612092
H    54     2.608019    -5.378821    -0.612092
H    55    -0.660022     5.814905    -2.942379
H    56     0.660022    -5.814905    -2.942379
H    57    -2.262564     5.104860    -3.087579
H    58     2.262564    -5.104860    -3.087579
H    59    -1.683666     7.951732    -2.101523
H    60     1.683666    -7.951732    -2.101523
H    61    -3.285702     7.239623    -2.242809
H    62     3.285702    -7.239623    -2.242809
H    63    -1.342549     7.670854    -4.578247
H    64     1.342549    -7.670854    -4.578247
H    65    -2.946324     6.962685    -4.717343
H    66     2.946324    -6.962685    -4.717343
H    67    -2.358843     9.810535    -3.744010
H    68     2.358843    -9.810535    -3.744010
H    69    -3.961875     9.103217    -3.878022
```

```
H     70      3.961875    -9.103217    -3.878022
H     71     -2.033234     9.559159    -6.238702
H     72      2.033234    -9.559159    -6.238702
H     73     -3.648233     8.847915    -6.372840
H     74      3.648233    -8.847915    -6.372840
H     75     -3.463481    10.535720    -5.872110
H     76      3.463481   -10.535720    -5.872110
S     77      6.390372     5.049005     0.525403
C     78      6.728927     6.662550     1.018958
C     79      5.633646     7.273261     1.575381
C     80      4.470479     6.452040     1.616757
H     81      7.717535     7.075507     0.868447
H     82      5.652869     8.286859     1.959717
C     83      3.185147     6.958706     2.219602
C     84      2.351644     7.835048     1.257164
C     85      1.103785     8.418625     1.932277
C     86      0.287423     9.336948     1.013592
C     87     -0.955971     9.929418     1.690698
C     88     -1.760123    10.858065     0.773465
H     89      2.572070     6.130181     2.587976
H     90      3.444179     7.561229     3.098727
H     91      2.058597     7.244888     0.378955
H     92      2.982250     8.651975     0.883616
H     93      0.464832     7.598507     2.290014
H     94      1.409396     8.981294     2.825894
H     95     -0.019947     8.777910     0.117988
H     96      0.929392    10.156014     0.658420
H     97     -1.601417     9.111558     2.039977
H     98     -0.647692    10.481205     2.589466
H     99     -2.110032    10.326255    -0.119243
H    100     -1.150816    11.705527     0.437261
H    101     -2.639316    11.262650     1.286684
S    102     -6.390372    -5.049005     0.525403
C    103     -6.728927    -6.662550     1.018958
C    104     -5.633646    -7.273261     1.575381
C    105     -4.470479    -6.452040     1.616757
H    106     -7.717535    -7.075507     0.868447
H    107     -5.652869    -8.286859     1.959717
C    108     -3.185147    -6.958706     2.219602
C    109     -2.351644    -7.835048     1.257164
C    110     -1.103785    -8.418625     1.932277
C    111     -0.287423    -9.336948     1.013592
C    112      0.955971    -9.929418     1.690698
C    113      1.760123   -10.858065     0.773465
H    114     -2.572070    -6.130181     2.587976
H    115     -3.444179    -7.561229     3.098727
H    116     -2.058597    -7.244888     0.378955
H    117     -2.982250    -8.651975     0.883616
H    118     -0.464832    -7.598507     2.290014
H    119     -1.409396    -8.981294     2.825894
H    120      0.019947    -8.777910     0.117988
```

```
H     121     -0.929392     -10.156014      0.658420
H     122      1.601417      -9.111558      2.039977
H     123      0.647692     -10.481205      2.589466
H     124      2.110032     -10.326255     -0.119243
H     125      1.150816     -11.705527      0.437261
H     126      2.639316     -11.262650      1.286684

T2-C
C       1     -0.606907      -0.336272      0.090865
C       2      0.606907       0.336272      0.090865
C       3     -1.676385       0.654534      0.042231
C       4      1.676385      -0.654534      0.042231
C       5      0.372454       1.747259      0.011610
C       6     -0.372454      -1.747259      0.011610
N       7     -1.002438       1.913606      0.022044
N       8      1.002438      -1.913606      0.022044
O       9     -2.897782       0.547591      0.031161
O      10      2.897782      -0.547591      0.031161
C      11      1.358714       2.751263     -0.117109
C      12     -1.358714      -2.751263     -0.117109
S      13      1.068208       4.437319     -0.549180
S      14     -1.068208      -4.437319     -0.549180
C      15      2.775341       4.806284     -0.532333
C      16     -2.775341      -4.806284     -0.532333
C      17      3.516803       3.667292     -0.176389
C      18     -3.516803      -3.667292     -0.176389
C      19      2.743071       2.533466      0.034323
C      20     -2.743071      -2.533466      0.034323
C      21      3.301048       6.112287     -0.820129
C      22     -3.301048      -6.112287     -0.820129
H      23      4.598007       3.671307     -0.112803
H      24     -4.598007      -3.671307     -0.112803
H      25      3.148151       1.556690      0.270203
H      26     -3.148151      -1.556690      0.270203
C      27     -1.773808       3.157058      0.175295
C      28      1.773808      -3.157058      0.175295
C      29     -1.685158       3.791038      1.583960
C      30      1.685158      -3.791038      1.583960
C      31     -2.341710       5.187223      1.533405
C      32      2.341710      -5.187223      1.533405
C      33     -2.216297       5.999202      2.830480
C      34      2.216297      -5.999202      2.830480
C      35     -2.788037       7.418557      2.708846
C      36      2.788037      -7.418557      2.708846
C      37     -2.667492       8.229865      4.004108
C      38      2.667492      -8.229865      4.004108
C      39     -2.243847       2.871419      2.695194
C      40      2.243847      -2.871419      2.695194
C      41     -3.763913       2.656702      2.699305
C      42      3.763913      -2.656702      2.699305
H      43     -2.804045       2.884148     -0.061166
```

```
H   44    2.804045   -2.884148   -0.061166
H   45   -1.456083    3.867447   -0.591256
H   46    1.456083   -3.867447   -0.591256
H   47   -3.082911    9.236341    3.884415
H   48    3.082911   -9.236341    3.884415
H   49   -0.621365    3.944239    1.811057
H   50    0.621365   -3.944239    1.811057
H   51   -3.402397    5.089491    1.264860
H   52    3.402397   -5.089491    1.264860
H   53   -1.875457    5.758692    0.718752
H   54    1.875457   -5.758692    0.718752
H   55   -2.729100    5.481147    3.651081
H   56    2.729100   -5.481147    3.651081
H   57   -1.156706    6.059569    3.118784
H   58    1.156706   -6.059569    3.118784
H   59   -3.844514    7.357469    2.413309
H   60    3.844514   -7.357469    2.413309
H   61   -2.272566    7.948467    1.896307
H   62    2.272566   -7.948467    1.896307
H   63   -3.204341    7.743043    4.826994
H   64    3.204341   -7.743043    4.826994
H   65   -1.619254    8.335531    4.308354
H   66    1.619254   -8.335531    4.308354
H   67   -1.939687    3.287980    3.662285
H   68    1.939687   -3.287980    3.662285
H   69   -1.741261    1.897931    2.630798
H   70    1.741261   -1.897931    2.630798
H   71   -4.307260    3.592742    2.864513
H   72    4.307260   -3.592742    2.864513
H   73   -4.118436    2.218737    1.761205
H   74    4.118436   -2.218737    1.761205
H   75   -4.043070    1.970524    3.505966
H   76    4.043070   -1.970524    3.505966
S   77    4.895297    6.516023   -0.174364
C   78    4.848576    8.071143   -0.911608
C   79    3.689491    8.273496   -1.617028
C   80    2.788037    7.170475   -1.579909
H   81    5.677136    8.754453   -0.780557
H   82    3.481989    9.185889   -2.164797
C   83    1.483270    7.204708   -2.334715
C   84    0.354936    7.962350   -1.599555
C   85   -0.922929    8.063592   -2.442428
C   86   -2.048508    8.845029   -1.752390
C   87   -3.325166    8.951876   -2.597469
C   88   -4.443341    9.741838   -1.907422
H   89    1.666619    7.704043   -3.294006
H   90    1.147377    6.191461   -2.577032
H   91    0.707970    8.969883   -1.344856
H   92    0.133314    7.462427   -0.647497
H   93   -0.683292    8.545317   -3.401117
H   94   -1.278533    7.052523   -2.687803
```

```
H     95    -1.690913     9.856131    -1.509596
H     96    -2.289478     8.366162    -0.792486
H     97    -3.082300     9.426162    -3.558384
H     98    -3.685112     7.941594    -2.836970
H     99    -4.124037    10.767343    -1.686435
H    100    -4.731918     9.272912    -0.959148
H    101    -5.338163     9.799787    -2.536697
S    102    -4.895297    -6.516023    -0.174364
C    103    -4.848576    -8.071143    -0.911608
C    104    -3.689491    -8.273496    -1.617028
C    105    -2.788037    -7.170475    -1.579909
H    106    -5.677136    -8.754453    -0.780557
H    107    -3.481989    -9.185889    -2.164797
C    108    -1.483270    -7.204708    -2.334715
C    109    -0.354936    -7.962350    -1.599555
C    110     0.922929    -8.063592    -2.442428
C    111     2.048508    -8.845029    -1.752390
C    112     3.325166    -8.951876    -2.597469
C    113     4.443341    -9.741838    -1.907422
H    114    -1.147377    -6.191461    -2.577032
H    115    -1.666619    -7.704043    -3.294006
H    116    -0.133314    -7.462427    -0.647497
H    117    -0.707970    -8.969883    -1.344856
H    118     1.278533    -7.052523    -2.687803
H    119     0.683292    -8.545317    -3.401117
H    120     2.289478    -8.366162    -0.792486
H    121     1.690913    -9.856131    -1.509596
H    122     3.685112    -7.941594    -2.836970
H    123     3.082300    -9.426162    -3.558384
H    124     4.731918    -9.272912    -0.959148
H    125     4.124037   -10.767343    -1.686435
H    126     5.338163    -9.799787    -2.536697

T3-B
C      1     0.412327     0.560372    -0.301971
C      2    -0.412327    -0.560372    -0.301971
C      3     1.795360     0.104638    -0.309479
C      4    -1.795360    -0.104638    -0.309479
C      5     0.387789    -1.745973    -0.308398
C      6    -0.387789     1.745973    -0.308398
N      7     1.708276    -1.315489    -0.316494
N      8    -1.708276     1.315489    -0.316494
O      9     2.868178     0.706515    -0.313904
O     10    -2.868178    -0.706515    -0.313904
C     11    -0.085663    -3.076467    -0.314555
C     12     0.085663     3.076467    -0.314555
S     13     0.909015    -4.536465    -0.324465
S     14    -0.909015     4.536465    -0.324465
C     15    -0.501700    -5.573467    -0.318181
C     16     0.501700     5.573467    -0.318181
C     17    -1.677357    -4.803507    -0.311341
```

```
C    18     1.677357     4.803507    -0.311341
C    19    -1.451434    -3.434590    -0.309307
C    20     1.451434     3.434590    -0.309307
C    21    -0.378283    -6.990663    -0.322338
C    22     0.378283     6.990663    -0.322338
H    23    -2.667493    -5.243496    -0.306106
H    24     2.667493     5.243496    -0.306106
H    25    -2.236931    -2.687227    -0.303765
H    26     2.236931     2.687227    -0.303765
C    27     2.945516    -2.104926    -0.289911
C    28    -2.945516     2.104926    -0.289911
C    29     3.402694    -2.477016     1.127321
C    30    -3.402694     2.477016     1.127321
C    31     4.713003    -3.274789     1.112491
C    32    -4.713003     3.274789     1.112491
C    33     5.208412    -3.642460     2.517607
C    34    -5.208412     3.642460     2.517607
C    35     6.520509    -4.437912     2.513007
C    36    -6.520509     4.437912     2.513007
C    37     7.017317    -4.808225     3.916686
C    38    -7.017317     4.808225     3.916686
C    39     8.330474    -5.602204     3.915210
C    40    -8.330474     5.602204     3.915210
C    41     8.818609    -5.969076     5.321543
C    42    -8.818609     5.969076     5.321543
H    43     3.702011    -1.479391    -0.769074
H    44    -3.702011     1.479391    -0.769074
H    45     2.817073    -2.985959    -0.922299
H    46    -2.817073     2.985959    -0.922299
H    47     3.535622    -1.553315     1.703360
H    48    -3.535622     1.553315     1.703360
H    49     2.621347    -3.057503     1.632693
H    50    -2.621347     3.057503     1.632693
H    51     5.487347    -2.690599     0.595838
H    52    -5.487347     2.690599     0.595838
H    53     4.574705    -4.193186     0.524345
H    54    -4.574705     4.193186     0.524345
H    55     5.344016    -2.722872     3.104494
H    56    -5.344016     2.722872     3.104494
H    57     4.432375    -4.225481     3.033986
H    58    -4.432375     4.225481     3.033986
H    59     7.295938    -3.853272     1.997170
H    60    -7.295938     3.853272     1.997170
H    61     6.385353    -5.356171     1.923054
H    62    -6.385353     5.356171     1.923054
H    63     7.151684    -3.890340     4.507559
H    64    -7.151684     3.890340     4.507559
H    65     6.242455    -5.393886     4.432896
H    66    -6.242455     5.393886     4.432896
H    67     9.105214    -5.016695     3.400928
H    68    -9.105214     5.016695     3.400928
```

```
H    69      8.197064     -6.519045      3.324201
H    70     -8.197064      6.519045      3.324201
H    71      8.993487     -5.070893      5.925963
H    72     -8.993487      5.070893      5.925963
H    73      8.079335     -6.584202      5.848612
H    74     -8.079335      6.584202      5.848612
H    75      9.756689     -6.533788      5.284899
H    76     -9.756689      6.533788      5.284899
S    77     -1.801752     -8.029404     -0.319908
C    78      0.782071     -7.767216     -0.327478
C    79      0.539383     -9.146334     -0.329388
C    80     -0.817316     -9.477026     -0.325902
H    81      1.326351     -9.891104     -0.334285
H    82      1.778331     -7.339657     -0.330421
S    83     -0.428057    -12.238810     -0.310945
C    84     -1.834093    -13.273983     -0.313454
C    85     -2.989190    -12.520211     -0.324447
C    86     -2.760749    -11.122459     -0.331682
C    87     -1.416665    -10.782627     -0.325519
H    88     -3.558063    -10.387246     -0.339746
H    89     -3.976646    -12.968226     -0.324820
C    90     -1.703563    -14.769476     -0.328525
C    91     -1.203800    -15.346644     -1.671341
C    92     -1.121720    -16.878098     -1.658924
C    93     -0.626143    -17.468621     -2.985637
C    94     -0.539383    -19.000767     -2.980148
C    95     -0.043057    -19.583215     -4.308666
H    96     -1.029045    -15.094127      0.474269
H    97     -2.690243    -15.187710     -0.098083
H    98     -0.214998    -14.928542     -1.900762
H    99     -1.876707    -15.016810     -2.473491
H   100     -0.453667    -17.198637     -0.846626
H   101     -2.112668    -17.292658     -1.424762
H   102      0.364169    -17.052063     -3.220546
H   103     -1.294618    -17.147783     -3.797752
H   104      0.128394    -19.321292     -2.168498
H   105     -1.528739    -19.417271     -2.745456
H   106      0.959073    -19.211221     -4.553541
H   107     -0.709863    -19.307958     -5.134618
H   108      0.007390    -20.676934     -4.271471
S   109      1.801752      8.029404     -0.319908
C   110     -0.782071      7.767216     -0.327478
C   111     -0.539383      9.146334     -0.329388
C   112      0.817316      9.477026     -0.325902
H   113     -1.326351      9.891104     -0.334285
H   114     -1.778331      7.339657     -0.330421
S   115      0.428057     12.238810     -0.310945
C   116      1.834093     13.273983     -0.313454
C   117      2.989190     12.520211     -0.324447
C   118      2.760749     11.122459     -0.331682
C   119      1.416665     10.782627     -0.325519
```

```
H    120     3.558063    10.387246    -0.339746
H    121     3.976646    12.968226    -0.324820
C    122     1.703563    14.769476    -0.328525
C    123     1.203800    15.346644    -1.671341
C    124     1.121720    16.878098    -1.658924
C    125     0.626143    17.468621    -2.985637
C    126     0.539383    19.000767    -2.980148
C    127     0.043057    19.583215    -4.308666
H    128     1.029045    15.094127     0.474269
H    129     2.690243    15.187710    -0.098083
H    130     0.214998    14.928542    -1.900762
H    131     1.876707    15.016810    -2.473491
H    132     0.453667    17.198637    -0.846626
H    133     2.112668    17.292658    -1.424762
H    134    -0.364169    17.052063    -3.220546
H    135     1.294618    17.147783    -3.797752
H    136    -0.128394    19.321292    -2.168498
H    137     1.528739    19.417271    -2.745456
H    138    -0.959073    19.211221    -4.553541
H    139     0.709863    19.307958    -5.134618
H    140    -0.007390    20.676934    -4.271471

T3-A
C      1    -0.399264    -0.569631    -0.030555
C      2     0.399264     0.569631    -0.030555
C      3    -1.793071    -0.147118    -0.066567
C      4     1.793071     0.147118    -0.066567
C      5    -0.427424     1.733977    -0.086774
C      6     0.427424    -1.733977    -0.086774
N      7    -1.740675     1.276228    -0.071079
N      8     1.740675    -1.276228    -0.071079
O      9    -2.846799    -0.780045    -0.085449
O     10     2.846799     0.780045    -0.085449
C     11     0.016632     3.070029    -0.202934
C     12    -0.016632    -3.070029    -0.202934
S     13    -1.003360     4.478746    -0.508345
S     14     1.003360    -4.478746    -0.508345
C     15     0.378863     5.553568    -0.530415
C     16    -0.378863    -5.553568    -0.530415
C     17     1.565062     4.832759    -0.310557
C     18    -1.565062    -4.832759    -0.310557
C     19     1.369015     3.470089    -0.136988
C     20    -1.369015    -3.470089    -0.136988
C     21     0.226091     6.949467    -0.757608
C     22    -0.226091    -6.949467    -0.757608
H     23     2.540788     5.302923    -0.280938
H     24    -2.540788    -5.302923    -0.280938
H     25     2.167707     2.755819     0.026582
H     26    -2.167707    -2.755819     0.026582
C     27    -2.984785     2.051714     0.029261
C     28     2.984785    -2.051714     0.029261
```

```
C    29    -3.259086     2.656209     1.427122
C    30     3.259086    -2.656209     1.427122
C    31    -4.457558     3.622284     1.312214
C    32     4.457558    -3.622284     1.312214
C    33    -4.771702     4.411124     2.591159
C    34     4.771702    -4.411124     2.591159
C    35    -5.894866     5.439904     2.399962
C    36     5.894866    -5.439904     2.399962
C    37    -6.216952     6.225909     3.676184
C    38     6.216952    -6.225909     3.676184
C    39    -3.417692     1.583679     2.530187
C    40     3.417692    -1.583679     2.530187
C    41    -4.690118     0.727021     2.468069
C    42     4.690118    -0.727021     2.468069
H    43    -3.778091     1.354726    -0.248330
H    44     3.778091    -1.354726    -0.248330
H    45    -2.974942     2.832903    -0.735152
H    46     2.974942    -2.832903    -0.735152
H    47    -7.019915     6.951384     3.506162
H    48     7.019915    -6.951384     3.506162
H    49    -2.384220     3.259757     1.704018
H    50     2.384220    -3.259757     1.704018
H    51    -5.352039     3.067930     0.997011
H    52     5.352039    -3.067930     0.997011
H    53    -4.248099     4.338489     0.505491
H    54     4.248099    -4.338489     0.505491
H    55    -5.055115     3.723772     3.398730
H    56     5.055115    -3.723772     3.398730
H    57    -3.862290     4.927677     2.931367
H    58     3.862290    -4.927677     2.931367
H    59    -6.800044     4.924587     2.050112
H    60     6.800044    -4.924587     2.050112
H    61    -5.612567     6.139507     1.601030
H    62     5.612567    -6.139507     1.601030
H    63    -6.538019     5.555900     4.482643
H    64     6.538019    -5.555900     4.482643
H    65    -5.338871     6.777403     4.033123
H    66     5.338871    -6.777403     4.033123
H    67    -3.376033     2.090360     3.501440
H    68     3.376033    -2.090360     3.501440
H    69    -2.538490     0.927218     2.508684
H    70     2.538490    -0.927218     2.508684
H    71    -5.594936     1.331598     2.589141
H    72     5.594936    -1.331598     2.589141
H    73    -4.768676     0.180644     1.523339
H    74     4.768676    -0.180644     1.523339
H    75    -4.682613    -0.014183     3.274460
H    76     4.682613     0.014183     3.274460
S    77     1.622414     8.022889    -0.819737
C    78    -0.947673     7.676983    -0.963500
C    79    -0.736468     9.046637    -1.162535
```

```
C     80      0.608506      9.419517    -1.116795
H     81     -1.537865      9.755318    -1.333835
H     82     -1.931167      7.221057    -0.966962
S     83      0.158481     12.126817    -1.615948
C     84      1.534358     13.200080    -1.666590
C     85      2.701202     12.501582    -1.435849
C     86      2.505328     11.116044    -1.217980
C     87      1.175285     10.729525    -1.279880
H     88      3.315599     10.422169    -1.023078
H     89      3.674102     12.980355    -1.426877
C     90      1.368722     14.672875    -1.905352
C     91      0.771490     15.442791    -0.706638
C     92      0.670548     16.950663    -0.968076
C     93      0.081723     17.732137     0.213867
C     94     -0.019663     19.242268    -0.039575
C     95     -0.608506     20.016255     1.145630
H     96      2.358379     15.080683    -2.141632
H     97      0.740124     14.840778    -2.789201
H     98      1.393493     15.260365     0.179240
H     99     -0.224665     15.042201    -0.477636
H    100      1.669596     17.345395    -1.202169
H    101      0.053672     17.123508    -1.861599
H    102      0.698024     17.556808     1.107620
H    103     -0.917728     17.337536     0.447946
H    104      0.978967     19.636500    -0.273508
H    105     -0.635261     19.417690    -0.932705
H    106      0.004833     19.887701     2.045569
H    107     -1.620961     19.667351     1.381859
H    108     -0.667018     21.089292     0.932763
S    109     -1.622414     -8.022889    -0.819737
C    110      0.947673     -7.676983    -0.963500
C    111      0.736468     -9.046637    -1.162535
C    112     -0.608506     -9.419517    -1.116795
H    113      1.537865     -9.755318    -1.333835
H    114      1.931167     -7.221057    -0.966962
S    115     -0.158481    -12.126817    -1.615948
C    116     -1.534358    -13.200080    -1.666590
C    117     -2.701202    -12.501582    -1.435849
C    118     -2.505328    -11.116044    -1.217980
C    119     -1.175285    -10.729525    -1.279880
H    120     -3.315599    -10.422169    -1.023078
H    121     -3.674102    -12.980355    -1.426877
C    122     -1.368722    -14.672875    -1.905352
C    123     -0.771490    -15.442791    -0.706638
C    124     -0.670548    -16.950663    -0.968076
C    125     -0.081723    -17.732137     0.213867
C    126      0.019663    -19.242268    -0.039575
C    127      0.608506    -20.016255     1.145630
H    128     -0.740124    -14.840778    -2.789201
H    129     -2.358379    -15.080683    -2.141632
H    130      0.224665    -15.042201    -0.477636
```

```
H   131   -1.393493   -15.260365    0.179240
H   132   -0.053672   -17.123508   -1.861599
H   133   -1.669596   -17.345395   -1.202169
H   134    0.917728   -17.337536    0.447946
H   135   -0.698024   -17.556808    1.107620
H   136    0.635261   -19.417690   -0.932705
H   137   -0.978967   -19.636500   -0.273508
H   138    1.620961   -19.667351    1.381859
H   139   -0.004833   -19.887701    2.045569
H   140    0.667018   -21.089292    0.932763
```

d) Anion-radical in dichloromethane calculated by PCM/B3LYP/6-31++G(d,p) method

```
T1-B
C    1   -0.711171   -0.016116   -1.417415
C    2    0.711171    0.016116   -1.417415
C    3   -1.188792    1.339981   -1.432145
C    4    1.188792   -1.339981   -1.432145
C    5    1.156676    1.359225   -1.442388
C    6   -1.156676   -1.359225   -1.442388
N    7   -0.021018    2.139502   -1.450537
N    8    0.021018   -2.139502   -1.450537
O    9   -2.342821    1.836064   -1.418761
O   10    2.342821   -1.836064   -1.418761
C   11    2.506831    1.829438   -1.498911
C   12   -2.506831   -1.829438   -1.498911
S   13    3.012475    3.516270   -1.729783
S   14   -3.012475   -3.516270   -1.729783
C   15    4.702436    3.091292   -1.694804
C   16   -4.702436   -3.091292   -1.694804
C   17    4.868243    1.738186   -1.523082
C   18   -4.868243   -1.738186   -1.523082
C   19    3.648967    1.023709   -1.414231
C   20   -3.648967   -1.023709   -1.414231
H   21    5.451865    3.864036   -1.797385
H   22   -5.451865   -3.864036   -1.797385
H   23    5.843291    1.264579   -1.472471
H   24   -5.843291   -1.264579   -1.472471
H   25    3.570782   -0.051025   -1.291934
H   26   -3.570782    0.051025   -1.291934
C   27   -0.149113    3.586587   -1.311397
C   28    0.149113   -3.586587   -1.311397
C   29    0.004145    4.083883    0.134426
C   30   -0.004145   -4.083883    0.134426
C   31   -0.153096    5.605627    0.244847
C   32    0.153096   -5.605627    0.244847
C   33   -0.021018    6.127570    1.681966
C   34    0.021018   -6.127570    1.681966
C   35   -0.172317    7.650144    1.798332
C   36    0.172317   -7.650144    1.798332
C   37   -0.038585    8.173116    3.234689
```

```
C   38    0.038585   -8.173116    3.234689
C   39   -0.187234    9.695866    3.352951
C   40    0.187234   -9.695866    3.352951
C   41   -0.051065   10.209060    4.791401
C   42    0.051065  -10.209060    4.791401
H   43   -1.151468    3.828414   -1.673882
H   44    1.151468   -3.828414   -1.673882
H   45    0.562460    4.085716   -1.974049
H   46   -0.562460   -4.085716   -1.974049
H   47   -0.750960    3.585529    0.755714
H   48    0.750960   -3.585529    0.755714
H   49    0.984837    3.785480    0.524997
H   50   -0.984837   -3.785480    0.524997
H   51   -1.132609    5.900509   -0.158690
H   52    1.132609   -5.900509   -0.158690
H   53    0.600837    6.095904   -0.388118
H   54   -0.600837   -6.095904   -0.388118
H   55   -0.776256    5.639104    2.314450
H   56    0.776256   -5.639104    2.314450
H   57    0.957080    5.829044    2.086068
H   58   -0.957080   -5.829044    2.086068
H   59   -1.150836    7.948537    1.394444
H   60    1.150836   -7.948537    1.394444
H   61    0.582502    8.138109    1.164375
H   62   -0.582502   -8.138109    1.164375
H   63   -0.793941    7.686844    3.869403
H   64    0.793941   -7.686844    3.869403
H   65    0.939421    7.874050    3.639686
H   66   -0.939421   -7.874050    3.639686
H   67   -1.164641    9.995268    2.949512
H   68    1.164641   -9.995268    2.949512
H   69    0.567298   10.182177    2.718948
H   70   -0.567298  -10.182177    2.718948
H   71   -0.814162    9.766156    5.442775
H   72    0.814162   -9.766156    5.442775
H   73    0.929939    9.954510    5.210489
H   74   -0.929939   -9.954510    5.210489
H   75   -0.162109   11.298030    4.840604
H   76    0.162109  -11.298030    4.840604

T1-A
C    1   -0.700177   -0.123094   -0.923180
C    2    0.700177    0.123094   -0.923180
C    3   -1.379270    1.144774   -0.958261
C    4    1.379270   -1.144774   -0.958261
C    5    0.936298    1.516122   -0.977235
C    6   -0.936298   -1.516122   -0.977235
N    7   -0.344801    2.113904   -0.970719
N    8    0.344801   -2.113904   -0.970719
O    9   -2.595408    1.453030   -0.957704
O   10    2.595408   -1.453030   -0.957704
```

```
C      11      2.195159      2.182136     -1.116773
C      12     -2.195159     -2.182136     -1.116773
S      13      2.414471      3.876145     -1.600270
S      14     -2.414471     -3.876145     -1.600270
C      15      4.151598      3.734862     -1.570778
C      16     -4.151598     -3.734862     -1.570778
C      17      4.538477      2.462778     -1.223838
C      18     -4.538477     -2.462778     -1.223838
C      19      3.452988      1.586397     -0.970942
C      20     -3.452988     -1.586397     -0.970942
H      21      4.764038      4.596745     -1.797573
H      22     -4.764038     -4.596745     -1.797573
H      23      5.578333      2.162728     -1.144774
H      24     -5.578333     -2.162728     -1.144774
H      25      3.552786      0.537622     -0.715718
H      26     -3.552786     -0.537622     -0.715718
C      27     -0.672563      3.524740     -0.782773
C      28      0.672563     -3.524740     -0.782773
C      29     -0.345057      4.091004      0.620590
C      30      0.345057     -4.091004      0.620590
C      31     -0.564800      5.618109      0.600682
C      32      0.564800     -5.618109      0.600682
C      33     -0.145783      6.350578      1.883082
C      34      0.145783     -6.350578      1.883082
C      35     -0.265501      7.876978      1.772292
C      36      0.265501     -7.876978      1.772292
C      37      0.145783      8.611709      3.053716
C      38     -0.145783     -8.611709      3.053716
C      39     -1.096330      3.360719      1.757466
C      40      1.096330     -3.360719      1.757466
C      41     -2.614031      3.584825      1.821889
C      42      2.614031     -3.584825      1.821889
H      43     -1.745389      3.597431     -0.978167
H      44      1.745389     -3.597431     -0.978167
H      45     -0.168974      4.124152     -1.547128
H      46      0.168974     -4.124152     -1.547128
H      47      0.050937      9.697489      2.940931
H      48     -0.050937     -9.697489      2.940931
H      49      0.725889      3.923246      0.797269
H      50     -0.725889     -3.923246      0.797269
H      51     -1.619452      5.839780      0.383992
H      52      1.619452     -5.839780      0.383992
H      53      0.008634      6.035032     -0.239293
H      54     -0.008634     -6.035032     -0.239293
H      55     -0.755352      6.008185      2.729881
H      56      0.755352     -6.008185      2.729881
H      57      0.893996      6.087322      2.126794
H      58     -0.893996     -6.087322      2.126794
H      59     -1.301675      8.140116      1.517343
H      60      1.301675     -8.140116      1.517343
H      61      0.353931      8.227884      0.935190
```

```
H    62   -0.353931   -8.227884    0.935190
H    63   -0.480276    8.308435    3.901582
H    64    0.480276   -8.308435    3.901582
H    65    1.187814    8.393437    3.316996
H    66   -1.187814   -8.393437    3.316996
H    67   -0.648621    3.661597    2.712972
H    68    0.648621   -3.661597    2.712972
H    69   -0.897572    2.286026    1.663637
H    70    0.897572   -2.286026    1.663637
H    71   -2.865970    4.638309    1.987682
H    72    2.865970   -4.638309    1.987682
H    73   -3.105459    3.251664    0.902886
H    74    3.105459   -3.251664    0.902886
H    75   -3.045206    3.012045    2.650860
H    76    3.045206   -3.012045    2.650860

T2-B
C     1   -0.401450   -0.584929   -0.245701
C     2    0.401450    0.584929   -0.245701
C     3   -1.782614   -0.180662   -0.255405
C     4    1.782614    0.180662   -0.255405
C     5   -0.428926    1.733366   -0.267873
C     6    0.428926   -1.733366   -0.267873
N     7   -1.749643    1.234177   -0.273747
N     8    1.749643   -1.234177   -0.273747
O     9   -2.856223   -0.826941   -0.239629
O    10    2.856223    0.826941   -0.239629
C    11   -0.021752    3.095540   -0.320728
C    12    0.021752   -3.095540   -0.320728
S    13   -1.096837    4.500425   -0.490029
S    14    1.096837   -4.500425   -0.490029
C    15    0.252231    5.637933   -0.476794
C    16   -0.252231   -5.637933   -0.476794
C    17    1.448374    4.940425   -0.354741
C    18   -1.448374   -4.940425   -0.354741
C    19    1.307731    3.545970   -0.270772
C    20   -1.307731   -3.545970   -0.270772
C    21    0.021752    7.054012   -0.581115
C    22   -0.021752   -7.054012   -0.581115
H    23    2.412514    5.437785   -0.324590
H    24   -2.412514   -5.437785   -0.324590
H    25    2.133233    2.848124   -0.183005
H    26   -2.133233   -2.848124   -0.183005
C    27   -3.000889    1.974968   -0.142378
C    28    3.000889   -1.974968   -0.142378
C    29   -3.334570    2.365470    1.305610
C    30    3.334570   -2.365470    1.305610
C    31   -4.667332    3.116827    1.413680
C    32    4.667332   -3.116827    1.413680
C    33   -5.032063    3.499059    2.854548
C    34    5.032063   -3.499059    2.854548
```

```
C    35    -6.364822     4.250370     2.972269
C    36     6.364822    -4.250370     2.972269
C    37    -6.729107     4.632165     4.413129
C    38     6.729107    -4.632165     4.413129
C    39    -8.061659     5.383457     4.534259
C    40     8.061659    -5.383457     4.534259
C    41    -8.416336     5.761062     5.977406
C    42     8.416336    -5.761062     5.977406
H    43    -3.777516     1.309664    -0.528063
H    44     3.777516    -1.309664    -0.528063
H    45    -2.978107     2.853374    -0.792064
H    46     2.978107    -2.853374    -0.792064
H    47    -3.372899     1.451144     1.911148
H    48     3.372899    -1.451144     1.911148
H    49    -2.527546     2.985085     1.715646
H    50     2.527546    -2.985085     1.715646
H    51    -5.470086     2.496633     0.989327
H    52     5.470086    -2.496633     0.989327
H    53    -4.623205     4.027109     0.798273
H    54     4.623205    -4.027109     0.798273
H    55    -5.074313     2.588551     3.469534
H    56     5.074313    -2.588551     3.469534
H    57    -4.228462     4.118527     3.278219
H    58     4.228462    -4.118527     3.278219
H    59    -7.168344     3.630541     2.548209
H    60     7.168344    -3.630541     2.548209
H    61    -6.322653     5.160890     2.356719
H    62     6.322653    -5.160890     2.356719
H    63    -6.771229     3.722135     5.029552
H    64     6.771229    -3.722135     5.029552
H    65    -5.925938     5.252232     4.837807
H    66     5.925938    -5.252232     4.837807
H    67    -8.864735     4.763999     4.111085
H    68     8.864735    -4.763999     4.111085
H    69    -8.020239     6.292947     3.918715
H    70     8.020239    -6.292947     3.918715
H    71    -8.498287     4.869219     6.610414
H    72     8.498287    -4.869219     6.610414
H    73    -7.648058     6.408996     6.416418
H    74     7.648058    -6.408996     6.416418
H    75    -9.371757     6.295047     6.028664
H    76     9.371757    -6.295047     6.028664
S    77     1.368992     8.196615    -0.580524
C    78     0.295617     9.581673    -0.727634
C    79    -1.010119     9.160027    -0.772389
C    80    -1.172740     7.746464    -0.691973
H    81    -2.139153     7.254559    -0.711758
H    82    -1.841250     9.852929    -0.858842
C    83     0.832875    10.982637    -0.803921
C    84     1.579957    11.314703    -2.113014
C    85     2.073582    12.766049    -2.163544
```

```
C     86     2.816341    13.112474    -3.460748
C     87     3.312216    14.563684    -3.516336
C     88     4.052628    14.901441    -4.815772
H     89    -0.017928    11.666133    -0.691361
H     90     1.501837    11.177965     0.045692
H     91     0.912225    11.120099    -2.962757
H     92     2.434019    10.634010    -2.227046
H     93     1.216441    13.444826    -2.044759
H     94     2.735427    12.954013    -1.305601
H     95     2.154645    12.924197    -4.318789
H     96     3.673309    12.433645    -3.580212
H     97     2.456124    15.242289    -3.396791
H     98     3.973993    14.751821    -2.659426
H     99     3.405197    14.755447    -5.688819
H    100     4.933691    14.261642    -4.946291
H    101     4.392851    15.942907    -4.823521
S    102    -1.368992    -8.196615    -0.580524
C    103    -0.295617    -9.581673    -0.727634
C    104     1.010119    -9.160027    -0.772389
C    105     1.172740    -7.746464    -0.691973
H    106     2.139153    -7.254559    -0.711758
H    107     1.841250    -9.852929    -0.858842
C    108    -0.832875   -10.982637    -0.803921
C    109    -1.579957   -11.314703    -2.113014
C    110    -2.073582   -12.766049    -2.163544
C    111    -2.816341   -13.112474    -3.460748
C    112    -3.312216   -14.563684    -3.516336
C    113    -4.052628   -14.901441    -4.815772
H    114    -1.501837   -11.177965     0.045692
H    115     0.017928   -11.666133    -0.691361
H    116    -2.434019   -10.634010    -2.227046
H    117    -0.912225   -11.120099    -2.962757
H    118    -2.735427   -12.954013    -1.305601
H    119    -1.216441   -13.444826    -2.044759
H    120    -3.673309   -12.433645    -3.580212
H    121    -2.154645   -12.924197    -4.318789
H    122    -3.973993   -14.751821    -2.659426
H    123    -2.456124   -15.242289    -3.396791
H    124    -4.933691   -14.261642    -4.946291
H    125    -3.405197   -14.755447    -5.688819
H    126    -4.392851   -15.942907    -4.823521
```

T2-A
```
C      1    -0.382457    -0.597167    -0.433755
C      2     0.382457     0.597167    -0.433755
C      3    -1.776958    -0.239354    -0.478761
C      4     1.776958     0.239354    -0.478761
C      5    -0.483572     1.715493    -0.497420
C      6     0.483572    -1.715493    -0.497420
N      7    -1.790355     1.178063    -0.496047
N      8     1.790355    -1.178063    -0.496047
```

```
O      9    -2.823396   -0.925687   -0.484745
O     10     2.823396    0.925687   -0.484745
C     11    -0.120621    3.085024   -0.631400
C     12     0.120621   -3.085024   -0.631400
S     13    -1.217731    4.403471   -1.093180
S     14     1.217731   -4.403471   -1.093180
C     15     0.077761    5.601370   -1.061848
C     16    -0.077761   -5.601370   -1.061848
C     17     1.276098    4.983387   -0.723639
C     18    -1.276098   -4.983387   -0.723639
C     19     1.176545    3.602090   -0.489194
C     20    -1.176545   -3.602090   -0.489194
C     21    -0.191316    6.984470   -1.353133
C     22     0.191316   -6.984470   -1.353133
H     23     2.210965    5.528622   -0.642865
H     24    -2.210965   -5.528622   -0.642865
H     25     2.013494    2.959383   -0.241841
H     26    -2.013494   -2.959383   -0.241841
C     27    -3.052740    1.894824   -0.328579
C     28     3.052740   -1.894824   -0.328579
C     29    -3.268988    2.516133    1.073057
C     30     3.268988   -2.516133    1.073057
C     31    -4.520732    3.416990    1.028202
C     32     4.520732   -3.416990    1.028202
C     33    -4.785308    4.221953    2.308356
C     34     4.785308   -4.221953    2.308356
C     35    -5.968086    5.191600    2.176858
C     36     5.968086   -5.191600    2.176858
C     37    -6.239122    5.993496    3.455339
C     38     6.239122   -5.993496    3.455339
C     39    -3.293379    1.461186    2.203351
C     40     3.293379   -1.461186    2.203351
C     41    -4.519688    0.538164    2.241713
C     42     4.519688   -0.538164    2.241713
H     43    -3.830903    1.157736   -0.541058
H     44     3.830903   -1.157736   -0.541058
H     45    -3.135568    2.672065   -1.093979
H     46     3.135568   -2.672065   -1.093979
H     47    -7.086721    6.676079    3.327749
H     48     7.086721   -6.676079    3.327749
H     49    -2.409678    3.169782    1.274202
H     50     2.409678   -3.169782    1.274202
H     51    -5.406712    2.811605    0.789735
H     52     5.406712   -2.811605    0.789735
H     53    -4.405015    4.122624    0.193610
H     54     4.405015   -4.122624    0.193610
H     55    -4.976380    3.542342    3.149457
H     56     4.976380   -3.542342    3.149457
H     57    -3.881001    4.789952    2.571564
H     58     3.881001   -4.789952    2.571564
H     59    -6.869703    4.626019    1.902767
```

```
H     60      6.869703     -4.626019      1.902767
H     61     -5.776526      5.883899      1.345291
H     62      5.776526     -5.883899      1.345291
H     63     -6.469394      5.329447      4.297256
H     64      6.469394     -5.329447      4.297256
H     65     -5.366143      6.594603      3.736906
H     66      5.366143     -6.594603      3.736906
H     67     -3.209717      1.984962      3.163763
H     68      3.209717     -1.984962      3.163763
H     69     -2.386875      0.848989      2.121732
H     70      2.386875     -0.848989      2.121732
H     71     -5.446783      1.096002      2.414345
H     72      5.446783     -1.096002      2.414345
H     73     -4.625457     -0.025708      1.310106
H     74      4.625457      0.025708      1.310106
H     75     -4.419857     -0.189040      3.055391
H     76      4.419857      0.189040      3.055391
S     77      1.095453      8.193220     -1.292533
C     78      0.002130      9.493016     -1.747784
C     79     -1.265563      8.997687     -1.927255
C     80     -1.382988      7.594164     -1.708841
H     81     -2.314595      7.049218     -1.815672
H     82     -2.100038      9.629015     -2.216138
C     83      0.483572     10.910285     -1.877106
C     84      0.866850     11.583699     -0.542300
C     85      1.311541     13.041041     -0.718276
C     86      1.693106     13.725529      0.600944
C     87      2.138054     15.184256      0.430311
C     88      2.517089     15.860656      1.753054
H     89      1.344797     10.956531     -2.558040
H     90     -0.319096     11.486556     -2.353944
H     91      1.672507     11.010910     -0.064153
H     92      0.006829     11.537822      0.138965
H     93      2.168140     13.078078     -1.406952
H     94      0.504206     13.610539     -1.201398
H     95      2.500409     13.156356      1.084467
H     96      0.836718     13.687801      1.289950
H     97      2.994117     15.222084     -0.257688
H     98      1.331575     15.753245     -0.052931
H     99      3.344409     15.333693      2.243463
H    100      1.670192     15.868457      2.449773
H    101      2.829496     16.899091      1.596502
S    102     -1.095453     -8.193220     -1.292533
C    103     -0.002130     -9.493016     -1.747784
C    104      1.265563     -8.997687     -1.927255
C    105      1.382988     -7.594164     -1.708841
H    106      2.314595     -7.049218     -1.815672
H    107      2.100038     -9.629015     -2.216138
C    108     -0.483572    -10.910285     -1.877106
C    109     -0.866850    -11.583699     -0.542300
C    110     -1.311541    -13.041041     -0.718276
```

```
C    111    -1.693106   -13.725529    0.600944
C    112    -2.138054   -15.184256    0.430311
C    113    -2.517089   -15.860656    1.753054
H    114     0.319096   -11.486556   -2.353944
H    115    -1.344797   -10.956531   -2.558040
H    116    -0.006829   -11.537822    0.138965
H    117    -1.672507   -11.010910   -0.064153
H    118    -0.504206   -13.610539   -1.201398
H    119    -2.168140   -13.078078   -1.406952
H    120    -0.836718   -13.687801    1.289950
H    121    -2.500409   -13.156356    1.084467
H    122    -1.331575   -15.753245   -0.052931
H    123    -2.994117   -15.222084   -0.257688
H    124    -1.670192   -15.868457    2.449773
H    125    -3.344409   -15.333693    2.243463
H    126    -2.829496   -16.899091    1.596502

T2-D
C      1     0.650792    -0.283719   -0.354452
C      2    -0.650792     0.283719   -0.354452
C      3     1.608152     0.790556   -0.374122
C      4    -1.608152    -0.790556   -0.374122
C      5    -0.554118     1.696063   -0.389313
C      6     0.554118    -1.696063   -0.389313
N      7     0.830471     1.973086   -0.401093
N      8    -0.830471    -1.973086   -0.401093
O      9     2.861713     0.809877   -0.355626
O     10    -2.861713    -0.809877   -0.355626
C     11    -1.622252     2.638250   -0.444526
C     12     1.622252    -2.638250   -0.444526
S     13    -1.459146     4.382143   -0.724850
S     14     1.459146    -4.382143   -0.724850
C     15    -3.205829     4.639555   -0.700854
C     16     3.205829    -4.639555   -0.700854
C     17    -3.844458     3.427200   -0.473191
C     18     3.844458    -3.427200   -0.473191
C     19    -2.985137     2.323187   -0.335661
C     20     2.985137    -2.323187   -0.335661
C     21    -3.805647     5.954557   -0.811722
C     22     3.805647    -5.954557   -0.811722
H     23    -4.925316     3.344700   -0.422537
H     24     4.925316    -3.344700   -0.422537
H     25    -3.315132     1.300589   -0.188971
H     26     3.315132    -1.300589   -0.188971
C     27     1.495300     3.264299   -0.250845
C     28    -1.495300    -3.264299   -0.250845
C     29     1.539270     3.769137    1.199571
C     30    -1.539270    -3.769137    1.199571
C     31     2.287192     5.102154    1.326943
C     32    -2.287192    -5.102154    1.326943
C     33     2.368586     5.618137    2.769961
```

```
C    34    -2.368586    -5.618137     2.769961
C    35     3.119696     6.949637     2.903082
C    36    -3.119696    -6.949637     2.903082
C    37     3.205829     7.465720     4.345552
C    38    -3.205829    -7.465720     4.345552
C    39     3.957500     8.796865     4.479918
C    40    -3.957500    -8.796865     4.479918
C    41     4.040180     9.304108     5.924518
C    42    -4.040180    -9.304108     5.924518
H    43     1.025142     4.000297    -0.907607
H    44    -1.025142    -4.000297    -0.907607
H    45     2.514472     3.113688    -0.615489
H    46    -2.514472    -3.113688    -0.615489
H    47     0.517320     3.880933     1.582571
H    48    -0.517320    -3.880933     1.582571
H    49     2.029458     3.006920     1.818423
H    50    -2.029458    -3.006920     1.818423
H    51     1.792839     5.858340     0.700134
H    52    -1.792839    -5.858340     0.700134
H    53     3.304716     4.987249     0.926154
H    54    -3.304716    -4.987249     0.926154
H    55     1.351180     5.734197     3.170420
H    56    -1.351180    -5.734197     3.170420
H    57     2.860740     4.860581     3.396777
H    58    -2.860740    -4.860581     3.396777
H    59     2.626414     7.707467     2.277033
H    60    -2.626414    -7.707467     2.277033
H    61     4.136247     6.833110     2.499677
H    62    -4.136247    -6.833110     2.499677
H    63     2.189666     7.583080     4.749901
H    64    -2.189666    -7.583080     4.749901
H    65     3.699008     6.708433     4.972587
H    66    -3.699008    -6.708433     4.972587
H    67     3.464269     9.554226     3.854713
H    68    -3.464269    -9.554226     3.854713
H    69     4.972617     8.680158     4.075347
H    70    -4.972617    -8.680158     4.075347
H    71     3.039938     9.462726     6.345380
H    72    -3.039938    -9.462726     6.345380
H    73     4.559150     8.582864     6.567362
H    74    -4.559150    -8.582864     6.567362
H    75     4.581844    10.254647     5.985146
H    76    -4.581844   -10.254647     5.985146
S    77    -5.287181     6.267406     0.102638
C    78    -5.408436     7.879763    -0.526671
C    79    -4.364266     8.162493    -1.363910
C    80    -3.440664     7.080256    -1.542359
H    81    -6.242080     8.511492    -0.251234
H    82    -4.255215     9.115815    -1.871477
C    83    -2.251965     7.200510    -2.466691
C    84    -1.054514     7.958773    -1.855968
```

```
C     85     0.115970     8.114012    -2.835302
C     86     1.312716     8.870212    -2.243285
C     87     2.483922     9.031198    -3.221832
C     88     3.674536     9.789140    -2.622662
H     89    -1.923029     6.207400    -2.790384
H     90    -2.572513     7.731241    -3.373428
H     91    -0.713374     7.431465    -0.955327
H     92    -1.388441     8.951297    -1.523970
H     93     0.444495     7.118931    -3.168120
H     94    -0.233992     8.638491    -3.736549
H     95     1.664479     8.344690    -1.343626
H     96     0.983550     9.864825    -1.908016
H     97     2.813994     8.037663    -3.555407
H     98     2.132670     9.555250    -4.121697
H     99     4.069274     9.270656    -1.740684
H    100     3.383408    10.799420    -2.310413
H    101     4.492020     9.886249    -3.345692
S    102     5.287181    -6.267406     0.102638
C    103     5.408436    -7.879763    -0.526671
C    104     4.364266    -8.162493    -1.363910
C    105     3.440664    -7.080256    -1.542359
H    106     6.242080    -8.511492    -0.251234
H    107     4.255215    -9.115815    -1.871477
C    108     2.251965    -7.200510    -2.466691
C    109     1.054514    -7.958773    -1.855968
C    110    -0.115970    -8.114012    -2.835302
C    111    -1.312716    -8.870212    -2.243285
C    112    -2.483922    -9.031198    -3.221832
C    113    -3.674536    -9.789140    -2.622662
H    114     1.923029    -6.207400    -2.790384
H    115     2.572513    -7.731241    -3.373428
H    116     0.713374    -7.431465    -0.955327
H    117     1.388441    -8.951297    -1.523970
H    118    -0.444495    -7.118931    -3.168120
H    119     0.233992    -8.638491    -3.736549
H    120    -1.664479    -8.344690    -1.343626
H    121    -0.983550    -9.864825    -1.908016
H    122    -2.813994    -8.037663    -3.555407
H    123    -2.132670    -9.555250    -4.121697
H    124    -4.069274    -9.270656    -1.740684
H    125    -3.383408   -10.799420    -2.310413
H    126    -4.492020    -9.886249    -3.345692

T2-C
C      1    -0.618476    -0.347968     0.246778
C      2     0.618476     0.347968     0.246778
C      3    -1.681657     0.622529     0.203542
C      4     1.681657    -0.622529     0.203542
C      5     0.378482     1.740628     0.183681
C      6    -0.378482    -1.740628     0.183681
N      7    -1.027872     1.880244     0.186417
```

```
N     8     1.027872    -1.880244     0.186417
O     9    -2.928428     0.506859     0.200975
O    10     2.928428    -0.506859     0.200975
C    11     1.341120     2.783562     0.047921
C    12    -1.341120    -2.783562     0.047921
S    13     0.989270     4.448249    -0.451545
S    14    -0.989270    -4.448249    -0.451545
C    15     2.694954     4.903872    -0.446128
C    16    -2.694954    -4.903872    -0.446128
C    17     3.461077     3.808874    -0.067570
C    18    -3.461077    -3.808874    -0.067570
C    19     2.727596     2.639013     0.200123
C    20    -2.727596    -2.639013     0.200123
C    21     3.144365     6.257232    -0.708433
C    22    -3.144365    -6.257232    -0.708433
H    23     4.543045     3.857189     0.000786
H    24    -4.543045    -3.857189     0.000786
H    25     3.168933     1.684201     0.462187
H    26    -3.168933    -1.684201     0.462187
C    27    -1.802348     3.104179     0.380252
C    28     1.802348    -3.104179     0.380252
C    29    -1.680410     3.736228     1.788465
C    30     1.680410    -3.736228     1.788465
C    31    -2.373611     5.114714     1.774227
C    32     2.373611    -5.114714     1.774227
C    33    -2.221690     5.929769     3.066224
C    34     2.221690    -5.929769     3.066224
C    35    -2.822933     7.338624     2.964747
C    36     2.822933    -7.338624     2.964747
C    37    -2.679378     8.152656     4.256195
C    38     2.679378    -8.152656     4.256195
C    39    -2.168782     2.797713     2.915947
C    40     2.168782    -2.797713     2.915947
C    41    -3.680263     2.532753     2.970416
C    42     3.680263    -2.532753     2.970416
H    43    -2.838752     2.822366     0.179643
H    44     2.838752    -2.822366     0.179643
H    45    -1.521704     3.839773    -0.379208
H    46     1.521704    -3.839773    -0.379208
H    47    -3.116344     9.151915     4.150472
H    48     3.116344    -9.151915     4.150472
H    49    -0.612599     3.915837     1.972581
H    50     0.612599    -3.915837     1.972581
H    51    -3.441846     4.991955     1.545776
H    52     3.441846    -4.991955     1.545776
H    53    -1.953173     5.699938     0.944466
H    54     1.953173    -5.699938     0.944466
H    55    -2.696704     5.401973     3.903795
H    56     2.696704    -5.401973     3.903795
H    57    -1.154450     6.010563     3.319479
H    58     1.154450    -6.010563     3.319479
```

```
H      59    -3.886662     7.258771     2.700081
H      60     3.886662    -7.258771     2.700081
H      61    -2.341333     7.878161     2.137586
H      62     2.341333    -7.878161     2.137586
H      63    -3.182078     7.655662     5.094692
H      64     3.182078    -7.655662     5.094692
H      65    -1.624528     8.277010     4.529163
H      66     1.624528    -8.277010     4.529163
H      67    -1.843921     3.217363     3.876169
H      68     1.843921    -3.217363     3.876169
H      69    -1.640951     1.841040     2.819309
H      70     1.640951    -1.841040     2.819309
H      71    -4.250982     3.451590     3.145395
H      72     4.250982    -3.451590     3.145395
H      73    -4.039565     2.074088     2.044367
H      74     4.039565    -2.074088     2.044367
H      75    -3.913132     1.842968     3.789558
H      76     3.913132    -1.842968     3.789558
S      77     4.552508     6.850491     0.182161
C      78     4.505897     8.377764    -0.639778
C      79     3.461077     8.432167    -1.521126
C      80     2.673927     7.234961    -1.578147
H      81     5.253008     9.131966    -0.432582
H      82     3.258112     9.297415    -2.144429
C      83     1.507780     7.099209    -2.528660
C      84     0.211016     7.775442    -2.035732
C      85    -0.942076     7.657700    -3.040635
C      86    -2.238271     8.327902    -2.565980
C      87    -3.393924     8.211560    -3.569053
C      88    -4.684912     8.883894    -3.087004
H      89     1.790986     7.550722    -3.489123
H      90     1.308025     6.041746    -2.731653
H      91     0.412794     8.835841    -1.831477
H      92    -0.088636     7.329001    -1.078423
H      93    -0.634092     8.102085    -3.998489
H      94    -1.137315     6.595100    -3.244608
H      95    -2.043480     9.391104    -2.361784
H      96    -2.546364     7.883515    -1.608469
H      97    -3.086689     8.654926    -4.526553
H      98    -3.589203     7.149515    -3.772092
H      99    -4.529839     9.954703    -2.907388
H     100    -5.035722     8.437926    -2.148581
H     101    -5.488545     8.782564    -3.824830
S     102    -4.552508    -6.850491     0.182161
C     103    -4.505897    -8.377764    -0.639778
C     104    -3.461077    -8.432167    -1.521126
C     105    -2.673927    -7.234961    -1.578147
H     106    -5.253008    -9.131966    -0.432582
H     107    -3.258112    -9.297415    -2.144429
C     108    -1.507780    -7.099209    -2.528660
C     109    -0.211016    -7.775442    -2.035732
```

```
C    110     0.942076    -7.657700    -3.040635
C    111     2.238271    -8.327902    -2.565980
C    112     3.393924    -8.211560    -3.569053
C    113     4.684912    -8.883894    -3.087004
H    114    -1.308025    -6.041746    -2.731653
H    115    -1.790986    -7.550722    -3.489123
H    116     0.088636    -7.329001    -1.078423
H    117    -0.412794    -8.835841    -1.831477
H    118     1.137315    -6.595100    -3.244608
H    119     0.634092    -8.102085    -3.998489
H    120     2.546364    -7.883515    -1.608469
H    121     2.043480    -9.391104    -2.361784
H    122     3.589203    -7.149515    -3.772092
H    123     3.086689    -8.654926    -4.526553
H    124     5.035722    -8.437926    -2.148581
H    125     4.529839    -9.954703    -2.907388
H    126     5.488545    -8.782564    -3.824830

T3-B
C      1    -0.708372     0.013765    -0.095498
C      2     0.708372    -0.013765    -0.095498
C      3    -1.130097     1.390637    -0.106318
C      4     1.130097    -1.390637    -0.106318
C      5     1.211615     1.311254    -0.114832
C      6    -1.211615    -1.311254    -0.114832
N      7     0.070080     2.140663    -0.122476
N      8    -0.070080    -2.140663    -0.122476
O      9    -2.258673     1.930925    -0.095645
O     10     2.258673    -1.930925    -0.095645
C     11     2.572488     1.717732    -0.157963
C     12    -2.572488    -1.717732    -0.157963
S     13     3.159771     3.388010    -0.299816
S     14    -3.159771    -3.388010    -0.299816
C     15     4.850391     2.880446    -0.282974
C     16    -4.850391    -2.880446    -0.282974
C     17     4.919834     1.492383    -0.179974
C     18    -4.919834    -1.492383    -0.179974
C     19     3.677734     0.849077    -0.112466
C     20    -3.677734    -0.849077    -0.112466
C     21     5.907408     3.842097    -0.368660
C     22    -5.907408    -3.842097    -0.368660
H     23     5.862958     0.956388    -0.151292
H     24    -5.862958    -0.956388    -0.151292
H     25     3.544642    -0.224741    -0.037829
H     26    -3.544642     0.224741    -0.037829
C     27    -0.000216     3.594885    -0.007600
C     28     0.000216    -3.594885    -0.007600
C     29     0.118164     4.104045     1.436973
C     30    -0.118164    -4.104045     1.436973
C     31     0.008504     5.631407     1.525412
C     32    -0.008504    -5.631407     1.525412
```

```
C    33     0.101431     6.163244     2.961968
C    34    -0.101431    -6.163244     2.961968
C    35    -0.008504     7.690674     3.059321
C    36     0.008504    -7.690674     3.059321
C    37     0.082847     8.222434     4.495767
C    38    -0.082847    -8.222434     4.495767
C    39    -0.027068     9.749749     4.596174
C    40     0.027068    -9.749749     4.596174
C    41     0.065236    10.271429     6.035040
C    42    -0.065236   -10.271429     6.035040
H    43    -0.975422     3.875291    -0.413557
H    44     0.975422    -3.875291    -0.413557
H    45     0.757518     4.049992    -0.649950
H    46    -0.757518    -4.049992    -0.649950
H    47    -0.675729     3.638835     2.034851
H    48     0.675729    -3.638835     2.034851
H    49     1.073358     3.777091     1.866032
H    50    -1.073358    -3.777091     1.866032
H    51    -0.944207     5.953813     1.081026
H    52     0.944207    -5.953813     1.081026
H    53     0.802484     6.089587     0.918015
H    54    -0.802484    -6.089587     0.918015
H    55    -0.692154     5.703796     3.568684
H    56     0.692154    -5.703796     3.568684
H    57     1.053722     5.839551     3.406196
H    58    -1.053722    -5.839551     3.406196
H    59    -0.960709     8.014022     2.613902
H    60     0.960709    -8.014022     2.613902
H    61     0.785469     8.150138     2.452534
H    62    -0.785469    -8.150138     2.452534
H    63    -0.710840     7.763302     5.103339
H    64     0.710840    -7.763302     5.103339
H    65     1.034966     7.899508     4.941950
H    66    -1.034966    -7.899508     4.941950
H    67    -0.978478    10.072903     4.151056
H    68     0.978478   -10.072903     4.151056
H    69     0.766021    10.209098     3.989746
H    70    -0.766021   -10.209098     3.989746
H    71    -0.735845     9.855718     6.658118
H    72     0.735845    -9.855718     6.658118
H    73     1.020869     9.993254     6.495638
H    74    -1.020869    -9.993254     6.495638
H    75    -0.016899    11.363455     6.071398
H    76     0.016899   -11.363455     6.071398
S    77     7.599489     3.332710    -0.377013
C    78     5.835054     5.227584    -0.456441
C    79     7.095543     5.865128    -0.528396
C    80     8.173184     4.997225    -0.498453
H    81     7.210269     6.941315    -0.601761
H    82     4.894851     5.767401    -0.468589
S    83    10.167464     6.951367    -0.641406
```

```
C     84    11.848044     6.443019    -0.667037
C     85    11.926187     5.073854    -0.606706
C     86    10.661098     4.420030    -0.541759
C     87     9.586668     5.289038    -0.551046
H     88    10.548832     3.342472    -0.489711
H     89    12.873649     4.544664    -0.606933
C     90    12.965768     7.442576    -0.762006
C     91    13.057678     8.173771    -2.117908
C     92    14.239576     9.148802    -2.187760
C     93    14.342373     9.885457    -3.529846
C     94    15.524188    10.861381    -3.606243
C     95    15.618350    11.594397    -4.949604
H     96    12.874147     8.188703     0.039183
H     97    13.903010     6.903271    -0.577721
H     98    12.122485     8.719478    -2.300626
H     99    13.143698     7.428015    -2.919212
H    100    14.150758     9.885173    -1.375830
H    101    15.174171     8.599342    -2.003468
H    102    13.407947    10.435433    -3.713923
H    103    14.429384     9.149073    -4.342034
H    104    15.437857    11.596730    -2.794194
H    105    16.458187    10.311896    -3.423677
H    106    14.712130    12.180504    -5.144277
H    107    15.739270    10.886517    -5.778426
H    108    16.471085    12.281981    -4.971384
S    109    -7.599489    -3.332710    -0.377013
C    110    -5.835054    -5.227584    -0.456441
C    111    -7.095543    -5.865128    -0.528396
C    112    -8.173184    -4.997225    -0.498453
H    113    -7.210269    -6.941315    -0.601761
H    114    -4.894851    -5.767401    -0.468589
S    115   -10.167464    -6.951367    -0.641406
C    116   -11.848044    -6.443019    -0.667037
C    117   -11.926187    -5.073854    -0.606706
C    118   -10.661098    -4.420030    -0.541759
C    119    -9.586668    -5.289038    -0.551046
H    120   -10.548832    -3.342472    -0.489711
H    121   -12.873649    -4.544664    -0.606933
C    122   -12.965768    -7.442576    -0.762006
C    123   -13.057678    -8.173771    -2.117908
C    124   -14.239576    -9.148802    -2.187760
C    125   -14.342373    -9.885457    -3.529846
C    126   -15.524188   -10.861381    -3.606243
C    127   -15.618350   -11.594397    -4.949604
H    128   -12.874147    -8.188703     0.039183
H    129   -13.903010    -6.903271    -0.577721
H    130   -12.122485    -8.719478    -2.300626
H    131   -13.143698    -7.428015    -2.919212
H    132   -14.150758    -9.885173    -1.375830
H    133   -15.174171    -8.599342    -2.003468
H    134   -13.407947   -10.435433    -3.713923
```

```
H    135   -14.429384   -9.149073   -4.342034
H    136   -15.437857  -11.596730   -2.794194
H    137   -16.458187  -10.311896   -3.423677
H    138   -14.712130  -12.180504   -5.144277
H    139   -15.739270  -10.886517   -5.778426
H    140   -16.471085  -12.281981   -4.971384

T3-A
C      1    -0.425014   -0.566566    0.099237
C      2     0.425014    0.566566    0.099237
C      3    -1.790105   -0.106351    0.056747
C      4     1.790105    0.106351    0.056747
C      5    -0.355895    1.746172    0.039969
C      6     0.355895   -1.746172    0.039969
N      7    -1.698763    1.308484    0.045632
N      8     1.698763   -1.308484    0.045632
O      9    -2.882096   -0.713981    0.048002
O     10     2.882096    0.713981    0.048002
C     11     0.107389    3.083025   -0.095067
C     12    -0.107389   -3.083025   -0.095067
S     13    -0.894125    4.483935   -0.525796
S     14     0.894125   -4.483935   -0.525796
C     15     0.490103    5.579262   -0.508463
C     16    -0.490103   -5.579262   -0.508463
C     17     1.646581    4.865786   -0.198956
C     18    -1.646581   -4.865786   -0.198956
C     19     1.445211    3.497519    0.024896
C     20    -1.445211   -3.497519    0.024896
C     21     0.325633    6.975066   -0.781909
C     22    -0.325633   -6.975066   -0.781909
H     23     2.621913    5.336760   -0.131545
H     24    -2.621913   -5.336760   -0.131545
H     25     2.234156    2.789625    0.252321
H     26    -2.234156   -2.789625    0.252321
C     27    -2.903193    2.115669    0.232890
C     28     2.903193   -2.115669    0.232890
C     29    -3.056388    2.740832    1.641098
C     30     3.056388   -2.740832    1.641098
C     31    -4.241912    3.728150    1.616697
C     32     4.241912   -3.728150    1.616697
C     33    -4.437993    4.536832    2.906747
C     34     4.437993   -4.536832    2.906747
C     35    -5.551835    5.587286    2.795639
C     36     5.551835   -5.587286    2.795639
C     37    -5.756307    6.391886    4.084731
C     38     5.756307   -6.391886    4.084731
C     39    -3.140032    1.683464    2.766216
C     40     3.140032   -1.683464    2.766216
C     41    -4.425855    0.845854    2.816163
C     42     4.425855   -0.845854    2.816163
H     43    -3.736118    1.439635    0.025727
```

H	44	3.736118	-1.439635	0.025727
H	45	-2.937771	2.901752	-0.527056
H	46	2.937771	-2.901752	-0.527056
H	47	-6.555403	7.132977	3.971592
H	48	6.555403	-7.132977	3.971592
H	49	-2.150944	3.331309	1.834861
H	50	2.150944	-3.331309	1.834861
H	51	-5.170470	3.189237	1.381014
H	52	5.170470	-3.189237	1.381014
H	53	-4.083767	4.431996	0.787532
H	54	4.083767	-4.431996	0.787532
H	55	-4.668346	3.863604	3.743109
H	56	4.668346	-3.863604	3.743109
H	57	-3.494185	5.038164	3.166656
H	58	3.494185	-5.038164	3.166656
H	59	-6.492562	5.088292	2.523744
H	60	6.492562	-5.088292	2.523744
H	61	-5.319656	6.273732	1.969586
H	62	5.319656	-6.273732	1.969586
H	63	-6.025508	5.736118	4.921570
H	64	6.025508	-5.736118	4.921570
H	65	-4.841511	6.927858	4.365025
H	66	4.841511	-6.927858	4.365025
H	67	-3.009481	2.195550	3.727636
H	68	3.009481	-2.195550	3.727636
H	69	-2.278037	1.011534	2.671650
H	70	2.278037	-1.011534	2.671650
H	71	-5.310849	1.465210	2.999433
H	72	5.310849	-1.465210	2.999433
H	73	-4.580425	0.292037	1.885420
H	74	4.580425	-0.292037	1.885420
H	75	-4.367096	0.112215	3.628010
H	76	4.367096	-0.112215	3.628010
S	77	1.713300	8.069003	-0.789760
C	78	-0.832980	7.686201	-1.072012
C	79	-0.619633	9.067238	-1.290689
C	80	0.702032	9.462052	-1.178437
H	81	-1.421442	9.759875	-1.523182
H	82	-1.810883	7.220721	-1.122886
S	83	0.290279	12.155450	-1.803235
C	84	1.661854	13.251097	-1.764694
C	85	2.799536	12.568253	-1.412745
C	86	2.593575	11.178823	-1.169102
C	87	1.282211	10.775457	-1.334128
H	88	3.388426	10.499655	-0.880314
H	89	3.767141	13.052811	-1.331024
C	90	1.502602	14.713463	-2.070714
C	91	0.718747	15.509460	-1.005913
C	92	0.619633	17.003930	-1.336453
C	93	-0.157023	17.809563	-0.286607
C	94	-0.259634	19.305616	-0.612627

```
C     95    -1.037326    20.103078     0.440955
H     96     2.508976    15.138137    -2.171157
H     97     1.011919    14.843815    -3.044962
H     98     1.206594    15.376297    -0.031260
H     99    -0.290971    15.089112    -0.908061
H    100     1.632240    17.420920    -1.436875
H    101     0.137901    17.127096    -2.317327
H    102     0.324587    17.686207     0.694379
H    103    -1.169478    17.392198    -0.185411
H    104     0.751878    19.723072    -0.713562
H    105    -0.740964    19.428950    -1.592785
H    106    -0.560462    20.027035     1.425582
H    107    -2.063845    19.730243     0.540465
H    108    -1.092489    21.165378     0.178511
S    109    -1.713300    -8.069003    -0.789760
C    110     0.832980    -7.686201    -1.072012
C    111     0.619633    -9.067238    -1.290689
C    112    -0.702032    -9.462052    -1.178437
H    113     1.421442    -9.759875    -1.523182
H    114     1.810883    -7.220721    -1.122886
S    115    -0.290279   -12.155450    -1.803235
C    116    -1.661854   -13.251097    -1.764694
C    117    -2.799536   -12.568253    -1.412745
C    118    -2.593575   -11.178823    -1.169102
C    119    -1.282211   -10.775457    -1.334128
H    120    -3.388426   -10.499655    -0.880314
H    121    -3.767141   -13.052811    -1.331024
C    122    -1.502602   -14.713463    -2.070714
C    123    -0.718747   -15.509460    -1.005913
C    124    -0.619633   -17.003930    -1.336453
C    125     0.157023   -17.809563    -0.286607
C    126     0.259634   -19.305616    -0.612627
C    127     1.037326   -20.103078     0.440955
H    128    -1.011919   -14.843815    -3.044962
H    129    -2.508976   -15.138137    -2.171157
H    130     0.290971   -15.089112    -0.908061
H    131    -1.206594   -15.376297    -0.031260
H    132    -0.137901   -17.127096    -2.317327
H    133    -1.632240   -17.420920    -1.436875
H    134     1.169478   -17.392198    -0.185411
H    135    -0.324587   -17.686207     0.694379
H    136     0.740964   -19.428950    -1.592785
H    137    -0.751878   -19.723072    -0.713562
H    138     2.063845   -19.730243     0.540465
H    139     0.560462   -20.027035     1.425582
H    140     1.092489   -21.165378     0.178511
```

e) Neutral molecule in chlorobenzene calculated by PCM/B3LYP/6-31++G(d,p) method

T1-B
```
C      1    -0.711581    -0.005120    -1.339141
```

```
C      2       0.711581      0.005120     -1.339141
C      3      -1.166960      1.363345     -1.351462
C      4       1.166960     -1.363345     -1.351462
C      5       1.166960      1.328675     -1.356995
C      6      -1.166960     -1.328675     -1.356995
N      7       0.032779      2.141111     -1.364351
N      8      -0.032779     -2.141111     -1.364351
O      9      -2.290626      1.880614     -1.350346
O     10       2.290626     -1.880614     -1.350346
C     11       2.542349      1.766696     -1.382221
C     12      -2.542349     -1.766696     -1.382221
S     13       3.098985      3.437119     -1.472968
S     14      -3.098985     -3.437119     -1.472968
C     15       4.753849      2.947386     -1.459736
C     16      -4.753849     -2.947386     -1.459736
C     17       4.885612      1.581647     -1.391325
C     18      -4.885612     -1.581647     -1.391325
C     19       3.639158      0.910298     -1.348301
C     20      -3.639158     -0.910298     -1.348301
H     21       5.531507      3.698085     -1.505111
H     22      -5.531507     -3.698085     -1.505111
H     23       5.843422      1.075216     -1.372061
H     24      -5.843422     -1.075216     -1.372061
H     25       3.524151     -0.166903     -1.298642
H     26      -3.524151      0.166903     -1.298642
C     27      -0.068611      3.600491     -1.304123
C     28       0.068611     -3.600491     -1.304123
C     29      -0.004717      4.162107      0.123697
C     30       0.004717     -4.162107      0.123697
C     31      -0.147016      5.689337      0.147601
C     32       0.147016     -5.689337      0.147601
C     33      -0.119663      6.275434      1.565601
C     34       0.119663     -6.275434      1.565601
C     35      -0.262936      7.802800      1.599156
C     36       0.262936     -7.802800      1.599156
C     37      -0.239988      8.389842      3.016599
C     38       0.239988     -8.389842      3.016599
C     39      -0.383524      9.917226      3.053310
C     40       0.383524     -9.917226      3.053310
C     41      -0.360212     10.494603      4.473459
C     42       0.360212    -10.494603      4.473459
H     43      -1.036523      3.843684     -1.749038
H     44       1.036523     -3.843684     -1.749038
H     45       0.696957      4.042714     -1.945281
H     46      -0.696957     -4.042714     -1.945281
H     47      -0.809039      3.704270      0.712522
H     48       0.809039     -3.704270      0.712522
H     49       0.941066      3.871251      0.597091
H     50      -0.941066     -3.871251      0.597091
H     51      -1.088250      5.973963     -0.343800
H     52       1.088250     -5.973963     -0.343800
```

```
H    53     0.660249     6.140598    -0.447049
H    54    -0.660249    -6.140598    -0.447049
H    55    -0.927266     5.822654     2.158419
H    56     0.927266    -5.822654     2.158419
H    57     0.820713     5.988462     2.057846
H    58    -0.820713    -5.988462     2.057846
H    59    -1.202450     8.088903     1.104333
H    60     1.202450    -8.088903     1.104333
H    61     0.545580     8.255588     1.006812
H    62    -0.545580    -8.255588     1.006812
H    63    -1.048544     7.937429     3.609330
H    64     1.048544    -7.937429     3.609330
H    65     0.699313     8.103919     3.512466
H    66    -0.699313    -8.103919     3.512466
H    67    -1.321987    10.203237     2.558224
H    68     1.321987   -10.203237     2.558224
H    69     0.424484    10.369890     2.461760
H    70    -0.424484   -10.369890     2.461760
H    71    -1.177947    10.086360     5.079523
H    72     1.177947   -10.086360     5.079523
H    73     0.580949    10.254221     4.982534
H    74    -0.580949   -10.254221     4.982534
H    75    -0.464823    11.585163     4.464133
H    76     0.464823   -11.585163     4.464133

T1-A
C     1    -0.709425     0.056213    -0.826698
C     2     0.709425    -0.056213    -0.826698
C     3    -1.048118     1.459414    -0.879585
C     4     1.048118    -1.459414    -0.879585
C     5     1.272610     1.219125    -0.907324
C     6    -1.272610    -1.219125    -0.907324
N     7     0.214848     2.132108    -0.906529
N     8    -0.214848    -2.132108    -0.906529
O     9    -2.126750     2.061454    -0.886149
O    10     2.126750    -2.061454    -0.886149
C    11     2.676639     1.533867    -1.029958
C    12    -2.676639    -1.533867    -1.029958
S    13     3.338253     3.081141    -1.550414
S    14    -3.338253    -3.081141    -1.550414
C    15     4.955083     2.480306    -1.470895
C    16    -4.955083    -2.480306    -1.470895
C    17     4.996790     1.166507    -1.071498
C    18    -4.996790    -1.166507    -1.071498
C    19     3.709885     0.625334    -0.827945
C    20    -3.709885    -0.625334    -0.827945
H    21     5.779066     3.133833    -1.724477
H    22    -5.779066    -3.133833    -1.724477
H    23     5.917503     0.606536    -0.957787
H    24    -5.917503    -0.606536    -0.957787
H    25     3.523101    -0.401487    -0.536663
```

```
H    26    -3.523101     0.401487    -0.536663
C    27     0.264915     3.592365    -0.789755
C    28    -0.264915    -3.592365    -0.789755
C    29     0.709425     4.118663     0.595738
C    30    -0.709425    -4.118663     0.595738
C    31     0.929145     5.642764     0.493801
C    32    -0.929145    -5.642764     0.493801
C    33     1.506293     6.296970     1.756938
C    34    -1.506293    -6.296970     1.756938
C    35     1.821478     7.787816     1.571044
C    36    -1.821478    -7.787816     1.571044
C    37     2.391729     8.446982     2.832333
C    38    -2.391729    -8.446982     2.832333
C    39    -0.243971     3.693624     1.737049
C    40     0.243971    -3.693624     1.737049
C    41    -1.632576     4.348732     1.742639
C    42     1.632576    -4.348732     1.742639
H    43    -0.749010     3.928961    -1.017427
H    44     0.749010    -3.928961    -1.017427
H    45     0.911783     3.994111    -1.574123
H    46    -0.911783    -3.994111    -1.574123
H    47     2.607559     9.508091     2.666056
H    48    -2.607559    -9.508091     2.666056
H    49     1.685446     3.667731     0.820631
H    50    -1.685446    -3.667731     0.820631
H    51    -0.015083     6.137133     0.226459
H    52     0.015083    -6.137133     0.226459
H    53     1.616690     5.835679    -0.341614
H    54    -1.616690    -5.835679    -0.341614
H    55     0.805239     6.184918     2.594392
H    56    -0.805239    -6.184918     2.594392
H    57     2.424408     5.767928     2.051723
H    58    -2.424408    -5.767928     2.051723
H    59     0.906787     8.314570     1.265398
H    60    -0.906787    -8.314570     1.265398
H    61     2.533822     7.906068     0.742779
H    62    -2.533822    -7.906068     0.742779
H    63     1.685848     8.377313     3.668641
H    64    -1.685848    -8.377313     3.668641
H    65     3.324296     7.961848     3.144753
H    66    -3.324296    -7.961848     3.144753
H    67     0.253812     3.903627     2.691364
H    68    -0.253812    -3.903627     2.691364
H    69    -0.361077     2.603116     1.703471
H    70     0.361077    -2.603116     1.703471
H    71    -1.571374     5.435260     1.866775
H    72     1.571374    -5.435260     1.866775
H    73    -2.183897     4.139796     0.820930
H    74     2.183897    -4.139796     0.820930
H    75    -2.228548     3.958539     2.574945
H    76     2.228548    -3.958539     2.574945
```

T2-B

C	1	-0.396545	-0.589600	-0.195062
C	2	0.396545	0.589600	-0.195062
C	3	-1.783474	-0.195698	-0.210499
C	4	1.783474	0.195698	-0.210499
C	5	-0.441108	1.714884	-0.221898
C	6	0.441108	-1.714884	-0.221898
N	7	-1.752093	1.231980	-0.229844
N	8	1.752093	-1.231980	-0.229844
O	9	-2.843391	-0.836023	-0.204118
O	10	2.843391	0.836023	-0.204118
C	11	-0.029609	3.090722	-0.260613
C	12	0.029609	-3.090722	-0.260613
S	13	-1.096336	4.489848	-0.403491
S	14	1.096336	-4.489848	-0.403491
C	15	0.249651	5.608262	-0.385008
C	16	-0.249651	-5.608262	-0.385008
C	17	1.447963	4.916413	-0.277149
C	18	-1.447963	-4.916413	-0.277149
C	19	1.295990	3.519609	-0.210047
C	20	-1.295990	-3.519609	-0.210047
C	21	0.029609	7.032640	-0.478061
C	22	-0.029609	-7.032640	-0.478061
H	23	2.412631	5.409886	-0.246064
H	24	-2.412631	-5.409886	-0.246064
H	25	2.120257	2.818989	-0.132601
H	26	-2.120257	-2.818989	-0.132601
C	27	-3.013392	1.970821	-0.154502
C	28	3.013392	-1.970821	-0.154502
C	29	-3.413476	2.359098	1.276366
C	30	3.413476	-2.359098	1.276366
C	31	-4.755408	3.101179	1.317171
C	32	4.755408	-3.101179	1.317171
C	33	-5.193987	3.477086	2.738921
C	34	5.193987	-3.477086	2.738921
C	35	-6.536422	4.218516	2.789391
C	36	6.536422	-4.218516	2.789391
C	37	-6.977287	4.592646	4.210672
C	38	6.977287	-4.592646	4.210672
C	39	-8.319884	5.333795	4.264347
C	40	8.319884	-5.333795	4.264347
C	41	-8.752243	5.703217	5.688205
C	42	8.752243	-5.703217	5.688205
H	43	-3.767599	1.302163	-0.576366
H	44	3.767599	-1.302163	-0.576366
H	45	-2.961380	2.844420	-0.808246
H	46	2.961380	-2.844420	-0.808246
H	47	-3.475438	1.444745	1.879246
H	48	3.475438	-1.444745	1.879246
H	49	-2.631629	2.983872	1.725374

```
H    50     2.631629    -2.983872     1.725374
H    51    -5.530548     2.475495     0.852308
H    52     5.530548    -2.475495     0.852308
H    53    -4.687227     4.012682     0.705960
H    54     4.687227    -4.012682     0.705960
H    55    -5.260926     2.564661     3.348572
H    56     5.260926    -2.564661     3.348572
H    57    -4.417338     4.101031     3.204141
H    58     4.417338    -4.101031     3.204141
H    59    -7.312178     3.594321     2.322503
H    60     7.312178    -3.594321     2.322503
H    61    -6.469292     5.131256     2.179408
H    62     6.469292    -5.131256     2.179408
H    63    -7.044534     3.680218     4.821188
H    64     7.044534    -3.680218     4.821188
H    65    -6.201841     5.216967     4.678438
H    66     6.201841    -5.216967     4.678438
H    67    -9.095020     4.710158     3.797584
H    68     9.095020    -4.710158     3.797584
H    69    -8.253149     6.245810     3.654805
H    70     8.253149    -6.245810     3.654805
H    71    -8.860968     4.808439     6.312893
H    72     8.860968    -4.808439     6.312893
H    73    -8.012910     6.354869     6.169313
H    74     8.012910    -6.354869     6.169313
H    75    -9.712805     6.230180     5.691036
H    76     9.712805    -6.230180     5.691036
S    77     1.382462     8.157541    -0.507478
C    78     0.320189     9.543535    -0.619528
C    79    -0.993855     9.137517    -0.632622
C    80    -1.162535     7.728073    -0.554144
H    81    -2.132499     7.242816    -0.549958
H    82    -1.819881     9.837932    -0.694446
C    83     0.864909    10.940613    -0.710562
C    84     1.545735    11.270821    -2.056257
C    85     2.042883    12.720014    -2.127200
C    86     2.720643    13.065119    -3.459852
C    87     3.218289    14.514672    -3.537964
C    88     3.894170    14.851485    -4.872251
H    89     0.027796    11.630362    -0.549250
H    90     1.578165    11.119666     0.104821
H    91     0.834341    11.081935    -2.870854
H    92     2.389124    10.585899    -2.214618
H    93     1.196044    13.402184    -1.963939
H    94     2.747961    12.902512    -1.303378
H    95     2.015862    12.880599    -4.283659
H    96     3.567953    12.383351    -3.623134
H    97     2.371647    15.195995    -3.375009
H    98     3.922525    14.699220    -2.714854
H    99     3.203674    14.709092    -5.712220
H   100     4.765527    14.209084    -5.047285
```

```
H    101    4.237079    15.891732    -4.895467
S    102   -1.382462    -8.157541    -0.507478
C    103   -0.320189    -9.543535    -0.619528
C    104    0.993855    -9.137517    -0.632622
C    105    1.162535    -7.728073    -0.554144
H    106    2.132499    -7.242816    -0.549958
H    107    1.819881    -9.837932    -0.694446
C    108   -0.864909   -10.940613    -0.710562
C    109   -1.545735   -11.270821    -2.056257
C    110   -2.042883   -12.720014    -2.127200
C    111   -2.720643   -13.065119    -3.459852
C    112   -3.218289   -14.514672    -3.537964
C    113   -3.894170   -14.851485    -4.872251
H    114   -1.578165   -11.119666     0.104821
H    115   -0.027796   -11.630362    -0.549250
H    116   -2.389124   -10.585899    -2.214618
H    117   -0.834341   -11.081935    -2.870854
H    118   -2.747961   -12.902512    -1.303378
H    119   -1.196044   -13.402184    -1.963939
H    120   -3.567953   -12.383351    -3.623134
H    121   -2.015862   -12.880599    -4.283659
H    122   -3.922525   -14.699220    -2.714854
H    123   -2.371647   -15.195995    -3.375009
H    124   -4.765527   -14.209084    -5.047285
H    125   -3.203674   -14.709092    -5.712220
H    126   -4.237079   -15.891732    -4.895467
```

T2-A
```
C      1   -0.363662    -0.610571    -0.283039
C      2    0.363662     0.610571    -0.283039
C      3   -1.771598    -0.295228    -0.334208
C      4    1.771598     0.295228    -0.334208
C      5   -0.533084     1.683279    -0.360745
C      6    0.533084    -1.683279    -0.360745
N      7   -1.819472     1.133396    -0.358017
N      8    1.819472    -1.133396    -0.358017
O      9   -2.788324    -0.999246    -0.341367
O     10    2.788324     0.999246    -0.341367
C     11   -0.197550     3.075019    -0.488171
C     12    0.197550    -3.075019    -0.488171
S     13   -1.307650     4.356691    -0.974273
S     14    1.307650    -4.356691    -0.974273
C     15   -0.045686     5.568286    -0.915648
C     16    0.045686    -5.568286    -0.915648
C     17    1.161619     4.988590    -0.552347
C     18   -1.161619    -4.988590    -0.552347
C     19    1.080926     3.602546    -0.321187
C     20   -1.080926    -3.602546    -0.321187
C     21   -0.332673     6.949804    -1.225845
C     22    0.332673    -6.949804    -1.225845
H     23    2.079679     5.555385    -0.447773
```

```
H    24    -2.079679    -5.555385    -0.447773
H    25     1.926397     2.979588    -0.053596
H    26    -1.926397    -2.979588    -0.053596
C    27    -3.106260     1.820973    -0.221795
C    28     3.106260    -1.820973    -0.221795
C    29    -3.367650     2.439685     1.172412
C    30     3.367650    -2.439685     1.172412
C    31    -4.643787     3.303926     1.094295
C    32     4.643787    -3.303926     1.094295
C    33    -4.961328     4.101657     2.366863
C    34     4.961328    -4.101657     2.366863
C    35    -6.167042     5.037775     2.204284
C    36     6.167042    -5.037775     2.204284
C    37    -6.491295     5.832219     3.474831
C    38     6.491295    -5.832219     3.474831
C    39    -3.386809     1.387916     2.306205
C    40     3.386809    -1.387916     2.306205
C    41    -4.581920     0.424255     2.318883
C    42     4.581920    -0.424255     2.318883
H    43    -3.858359     1.062147    -0.449337
H    44     3.858359    -1.062147    -0.449337
H    45    -3.189668     2.586941    -0.997553
H    46     3.189668    -2.586941    -0.997553
H    47    -7.354107     6.490592     3.325382
H    48     7.354107    -6.490592     3.325382
H    49    -2.532678     3.118894     1.391493
H    50     2.532678    -3.118894     1.391493
H    51    -5.505226     2.672513     0.836019
H    52     5.505226    -2.672513     0.836019
H    53    -4.529174     4.011487     0.261128
H    54     4.529174    -4.011487     0.261128
H    55    -5.154820     3.417168     3.203175
H    56     5.154820    -3.417168     3.203175
H    57    -4.079933     4.694421     2.652208
H    58     4.079933    -4.694421     2.652208
H    59    -7.045269     4.446985     1.908891
H    60     7.045269    -4.446985     1.908891
H    61    -5.974598     5.734550     1.376666
H    62     5.974598    -5.734550     1.376666
H    63    -6.723875     5.162468     4.311408
H    64     6.723875    -5.162468     4.311408
H    65    -5.642779     6.457636     3.777289
H    66     5.642779    -6.457636     3.777289
H    67    -3.346563     1.920247     3.264154
H    68     3.346563    -1.920247     3.264154
H    69    -2.457159     0.807178     2.256467
H    70     2.457159    -0.807178     2.256467
H    71    -5.531356     0.952595     2.457317
H    72     5.531356    -0.952595     2.457317
H    73    -4.643932    -0.156013     1.393397
H    74     4.643932     0.156013     1.393397
```

```
H     75    -4.481538    -0.288188     3.145044
H     76     4.481538     0.288188     3.145044
S     77     0.963955     8.126132    -1.401288
C     78    -0.161480     9.421887    -1.743282
C     79    -1.452917     8.949470    -1.722638
C     80    -1.554765     7.561378    -1.431960
H     81    -2.499450     7.032285    -1.369743
H     82    -2.309590     9.587464    -1.911649
C     83     0.312547    10.825596    -1.991864
C     84     0.881771    11.536202    -0.745346
C     85     1.307650    12.981553    -1.031733
C     86     1.878062    13.701579     0.197358
C     87     2.305059    15.148781    -0.082310
C     88     2.875354    15.860408     1.150161
H     89     1.072576    10.830476    -2.784465
H     90    -0.541588    11.395919    -2.376287
H     91     1.742099    10.969676    -0.365294
H     92     0.124525    11.522637     0.049479
H     93     2.057898    12.986163    -1.835618
H     94     0.444225    13.545146    -1.413778
H     95     2.741678    13.137996     0.579374
H     96     1.128222    13.695533     1.001801
H     97     3.053657    15.154980    -0.886717
H     98     1.442013    15.712480    -0.462997
H     99     3.760538    15.338765     1.533437
H    100     2.137542    15.900030     1.960514
H    101     3.169928    16.889559     0.917141
S    102    -0.963955    -8.126132    -1.401288
C    103     0.161480    -9.421887    -1.743282
C    104     1.452917    -8.949470    -1.722638
C    105     1.554765    -7.561378    -1.431960
H    106     2.499450    -7.032285    -1.369743
H    107     2.309590    -9.587464    -1.911649
C    108    -0.312547   -10.825596    -1.991864
C    109    -0.881771   -11.536202    -0.745346
C    110    -1.307650   -12.981553    -1.031733
C    111    -1.878062   -13.701579     0.197358
C    112    -2.305059   -15.148781    -0.082310
C    113    -2.875354   -15.860408     1.150161
H    114     0.541588   -11.395919    -2.376287
H    115    -1.072576   -10.830476    -2.784465
H    116    -0.124525   -11.522637     0.049479
H    117    -1.742099   -10.969676    -0.365294
H    118    -0.444225   -13.545146    -1.413778
H    119    -2.057898   -12.986163    -1.835618
H    120    -1.128222   -13.695533     1.001801
H    121    -2.741678   -13.137996     0.579374
H    122    -1.442013   -15.712480    -0.462997
H    123    -3.053657   -15.154980    -0.886717
H    124    -2.137542   -15.900030     1.960514
H    125    -3.760538   -15.338765     1.533437
```

```
H    126   -3.169928   -16.889559    0.917141


T2-D
C      1    0.651086   -0.285784   -0.256700
C      2   -0.651086    0.285784   -0.256700
C      3    1.611756    0.790161   -0.284752
C      4   -1.611756   -0.790161   -0.284752
C      5   -0.545677    1.681992   -0.303969
C      6    0.545677   -1.681992   -0.303969
N      7    0.819202    1.978627   -0.317934
N      8   -0.819202   -1.978627   -0.317934
O      9    2.848889    0.816815   -0.272293
O     10   -2.848889   -0.816815   -0.272293
C     11   -1.630929    2.625749   -0.354719
C     12    1.630929   -2.625749   -0.354719
S     13   -1.483662    4.360355   -0.625826
S     14    1.483662   -4.360355   -0.625826
C     15   -3.218165    4.589322   -0.601981
C     16    3.218165   -4.589322   -0.601981
C     17   -3.854575    3.378035   -0.371938
C     18    3.854575   -3.378035   -0.371938
C     19   -2.977151    2.285209   -0.240436
C     20    2.977151   -2.285209   -0.240436
C     21   -3.833520    5.898284   -0.744763
C     22    3.833520   -5.898284   -0.744763
H     23   -4.933432    3.285388   -0.324837
H     24    4.933432   -3.285388   -0.324837
H     25   -3.297610    1.259834   -0.093199
H     26    3.297610   -1.259834   -0.093199
C     27    1.483662    3.279026   -0.212765
C     28   -1.483662   -3.279026   -0.212765
C     29    1.556770    3.815365    1.224321
C     30   -1.556770   -3.815365    1.224321
C     31    2.289343    5.161022    1.299883
C     32   -2.289343   -5.161022    1.299883
C     33    2.406951    5.705139    2.730026
C     34   -2.406951   -5.705139    2.730026
C     35    3.140333    7.050413    2.813640
C     36   -3.140333   -7.050413    2.813640
C     37    3.263553    7.594607    4.242997
C     38   -3.263553   -7.594607    4.242997
C     39    3.997147    8.939777    4.328550
C     40   -3.997147   -8.939777    4.328550
C     41    4.116700    9.475508    5.760146
C     42   -4.116700   -9.475508    5.760146
H     43    0.997727    3.991718   -0.882858
H     44   -0.997727   -3.991718   -0.882858
H     45    2.493815    3.119366   -0.597118
H     46   -2.493815   -3.119366   -0.597118
H     47    0.544760    3.922156    1.633925
H     48   -0.544760   -3.922156    1.633925
```

```
H     49      2.074761      3.074191      1.845502
H     50     -2.074761     -3.074191      1.845502
H     51      1.764674      5.897450      0.674395
H     52     -1.764674     -5.897450      0.674395
H     53      3.295228      5.051565      0.870167
H     54     -3.295228     -5.051565      0.870167
H     55      1.400862      5.813006      3.160105
H     56     -1.400862     -5.813006      3.160105
H     57      2.930693      4.967416      3.354595
H     58     -2.930693     -4.967416      3.354595
H     59      2.615278      7.788403      2.189842
H     60     -2.615278     -7.788403      2.189842
H     61      4.145206      6.941992      2.380156
H     62     -4.145206     -6.941992      2.380156
H     63      2.258971      7.703401      4.677502
H     64     -2.258971     -7.703401      4.677502
H     65      3.788698      6.857151      4.867595
H     66     -3.788698     -6.857151      4.867595
H     67      3.472231      9.677179      3.705346
H     68     -3.472231     -9.677179      3.705346
H     69      5.000787      8.831503      3.894230
H     70     -5.000787     -8.831503      3.894230
H     71      3.127788      9.626553      6.209515
H     72     -3.127788     -9.626553      6.209515
H     73      4.667307      8.775060      6.399577
H     74     -4.667307     -8.775060      6.399577
H     75      4.644416     10.435311      5.785757
H     76     -4.644416    -10.435311      5.785757
S     77     -5.300718      6.221264      0.176778
C     78     -5.441326      7.805328     -0.502697
C     79     -4.420393      8.070458     -1.374124
C     80     -3.488802      6.992809     -1.527959
H     81     -6.266513      8.445193     -0.220387
H     82     -4.330970      9.006984     -1.914384
C     83     -2.315078      7.091794     -2.472453
C     84     -1.125574      7.895780     -1.905414
C     85      0.035234      8.020039     -2.900526
C     86      1.224696      8.820313     -2.353597
C     87      2.386697      8.950402     -3.347622
C     88      3.569443      9.754155     -2.794631
H     89     -1.973110      6.092517     -2.761247
H     90     -2.657608      7.579496     -3.394365
H     91     -0.770522      7.418395     -0.982463
H     92     -1.472166      8.897607     -1.618791
H     93      0.375530      7.015007     -3.188835
H     94     -0.328841      8.496040     -3.822522
H     95      1.590050      8.343780     -1.432243
H     96      0.883458      9.824938     -2.064016
H     97      2.729389      7.946778     -3.635295
H     98      2.021528      9.424786     -4.269091
H     99      3.977925      9.285744     -1.891170
```

```
H    100     3.265166   10.774063   -2.530324
H    101     4.380413    9.827727   -3.527518
S    102     5.300718   -6.221264    0.176778
C    103     5.441326   -7.805328   -0.502697
C    104     4.420393   -8.070458   -1.374124
C    105     3.488802   -6.992809   -1.527959
H    106     6.266513   -8.445193   -0.220387
H    107     4.330970   -9.006984   -1.914384
C    108     2.315078   -7.091794   -2.472453
C    109     1.125574   -7.895780   -1.905414
C    110    -0.035234   -8.020039   -2.900526
C    111    -1.224696   -8.820313   -2.353597
C    112    -2.386697   -8.950402   -3.347622
C    113    -3.569443   -9.754155   -2.794631
H    114     1.973110   -6.092517   -2.761247
H    115     2.657608   -7.579496   -3.394365
H    116     0.770522   -7.418395   -0.982463
H    117     1.472166   -8.897607   -1.618791
H    118    -0.375530   -7.015007   -3.188835
H    119     0.328841   -8.496040   -3.822522
H    120    -1.590050   -8.343780   -1.432243
H    121    -0.883458   -9.824938   -2.064016
H    122    -2.729389   -7.946778   -3.635295
H    123    -2.021528   -9.424786   -4.269091
H    124    -3.977925   -9.285744   -1.891170
H    125    -3.265166  -10.774063   -2.530324
H    126    -4.380413   -9.827727   -3.527518

T2-C
C      1    -0.616162   -0.355015    0.413138
C      2     0.616162    0.355015    0.413138
C      3    -1.690512    0.608969    0.355914
C      4     1.690512   -0.608969    0.355914
C      5     0.358017    1.726336    0.325054
C      6    -0.358017   -1.726336    0.325054
N      7    -1.032246    1.878090    0.324554
N      8     1.032246   -1.878090    0.324554
O      9    -2.920868    0.491966    0.351023
O     10     2.920868   -0.491966    0.351023
C     11     1.332080    2.778733    0.196178
C     12    -1.332080   -2.778733    0.196178
S     13     0.998013    4.420813   -0.343913
S     14    -0.998013   -4.420813   -0.343913
C     15     2.692084    4.858082   -0.307139
C     16    -2.692084   -4.858082   -0.307139
C     17     3.452768    3.780685    0.123239
C     18    -3.452768   -3.780685    0.123239
C     19     2.701072    2.620662    0.393721
C     20    -2.701072   -2.620662    0.393721
C     21     3.157247    6.196842   -0.631004
C     22    -3.157247   -6.196842   -0.631004
```

```
H    23     4.531804     3.827238     0.214043
H    24    -4.531804    -3.827238     0.214043
H    25     3.131754     1.671608     0.690633
H    26    -3.131754    -1.671608     0.690633
C    27    -1.815181     3.109238     0.464024
C    28     1.815181    -3.109238     0.464024
C    29    -1.724583     3.782060     1.854531
C    30     1.724583    -3.782060     1.854531
C    31    -2.411266     5.161917     1.776250
C    32     2.411266    -5.161917     1.776250
C    33    -2.289215     6.017055     3.045300
C    34     2.289215    -6.017055     3.045300
C    35    -2.879839     7.424367     2.880262
C    36     2.879839    -7.424367     2.880262
C    37    -2.767837     8.279494     4.147890
C    38     2.767837    -8.279494     4.147890
C    39    -2.247519     2.880462     2.997090
C    40     2.247519    -2.880462     2.997090
C    41    -3.761437     2.626208     3.023850
C    42     3.761437    -2.626208     3.023850
H    43    -2.845062     2.815865     0.248423
H    44     2.845062    -2.815865     0.248423
H    45    -1.520520     3.814789    -0.317341
H    46     1.520520    -3.814789    -0.317341
H    47    -3.196223     9.276403     3.996639
H    48     3.196223    -9.276403     3.996639
H    49    -0.661455     3.963982     2.062603
H    50     0.661455    -3.963982     2.062603
H    51    -3.473153     5.034805     1.523663
H    52     3.473153    -5.034805     1.523663
H    53    -1.967207     5.718901     0.939345
H    54     1.967207    -5.718901     0.939345
H    55    -2.790044     5.519080     3.885856
H    56     2.790044    -5.519080     3.885856
H    57    -1.228867     6.101059     3.324894
H    58     1.228867    -6.101059     3.324894
H    59    -3.936021     7.340450     2.588609
H    60     3.936021    -7.340450     2.588609
H    61    -2.372383     7.934144     2.049699
H    62     2.372383    -7.934144     2.049699
H    63    -3.296797     7.813023     4.987618
H    64     3.296797    -7.813023     4.987618
H    65    -1.720509     8.408289     4.446380
H    66     1.720509    -8.408289     4.446380
H    67    -1.943566     3.329541     3.950245
H    68     1.943566    -3.329541     3.950245
H    69    -1.722351     1.918269     2.948057
H    70     1.722351    -1.918269     2.948057
H    71    -4.329145     3.553181     3.158639
H    72     4.329145    -3.553181     3.158639
H    73    -4.107881     2.142553     2.105606
```

```
H     74      4.107881     -2.142553      2.105606
H     75     -4.016281      1.963382      3.858044
H     76      4.016281     -1.963382      3.858044
S     77      4.520667      6.838056      0.282980
C     78      4.510959      8.305664     -0.632070
C     79      3.517174      8.304472     -1.572470
C     80      2.730430      7.106996     -1.589544
H     81      5.237147      9.079742     -0.423488
H     82      3.348545      9.129122     -2.257012
C     83      1.610498      6.910213     -2.582832
C     84      0.300718      7.630790     -2.198171
C     85     -0.804237      7.452058     -3.247073
C     86     -2.111512      8.169182     -2.884959
C     87     -3.218896      7.993291     -3.932806
C     88     -4.520667      8.715025     -3.565164
H     89      1.945395      7.292176     -3.556004
H     90      1.409595      5.843023     -2.723290
H     91      0.505377      8.700680     -2.058868
H     92     -0.049276      7.256317     -1.227037
H     93     -0.444170      7.822878     -4.217692
H     94     -1.004237      6.379594     -3.384182
H     95     -1.910919      9.241924     -2.748602
H     96     -2.471856      7.799356     -1.913995
H     97     -2.858598      8.361472     -4.903452
H     98     -3.420736      6.921631     -4.067836
H     99     -4.357529      9.794086     -3.457035
H    100     -4.923667      8.344081     -2.615127
H    101     -5.288987      8.569415     -4.332422
S    102     -4.520667     -6.838056      0.282980
C    103     -4.510959     -8.305664     -0.632070
C    104     -3.517174     -8.304472     -1.572470
C    105     -2.730430     -7.106996     -1.589544
H    106     -5.237147     -9.079742     -0.423488
H    107     -3.348545     -9.129122     -2.257012
C    108     -1.610498     -6.910213     -2.582832
C    109     -0.300718     -7.630790     -2.198171
C    110      0.804237     -7.452058     -3.247073
C    111      2.111512     -8.169182     -2.884959
C    112      3.218896     -7.993291     -3.932806
C    113      4.520667     -8.715025     -3.565164
H    114     -1.409595     -5.843023     -2.723290
H    115     -1.945395     -7.292176     -3.556004
H    116      0.049276     -7.256317     -1.227037
H    117     -0.505377     -8.700680     -2.058868
H    118      1.004237     -6.379594     -3.384182
H    119      0.444170     -7.822878     -4.217692
H    120      2.471856     -7.799356     -1.913995
H    121      1.910919     -9.241924     -2.748602
H    122      3.420736     -6.921631     -4.067836
H    123      2.858598     -8.361472     -4.903452
H    124      4.923667     -8.344081     -2.615127
```

```
H    125     4.357529    -9.794086    -3.457035
H    126     5.288987    -8.569415    -4.332422

T3-B
C      1    -0.428791    -0.566089    -0.166481
C      2     0.428791     0.566089    -0.166481
C      3    -1.791815    -0.094818    -0.184047
C      4     1.791815     0.094818    -0.184047
C      5    -0.344406     1.737063    -0.194466
C      6     0.344406    -1.737063    -0.194466
N      7    -1.680606     1.328368    -0.203582
N      8     1.680606    -1.328368    -0.203582
O      9    -2.885499    -0.675344    -0.179627
O     10     2.885499     0.675344    -0.179627
C     11     0.144028     3.086708    -0.232015
C     12    -0.144028    -3.086708    -0.232015
S     13    -0.842263     4.543552    -0.372399
S     14     0.842263    -4.543552    -0.372399
C     15     0.566024     5.583876    -0.359367
C     16    -0.566024    -5.583876    -0.359367
C     17     1.724012     4.824336    -0.248326
C     18    -1.724012    -4.824336    -0.248326
C     19     1.492660     3.439845    -0.179647
C     20    -1.492660    -3.439845    -0.179647
C     21     0.428791     7.014859    -0.455875
C     22    -0.428791    -7.014859    -0.455875
H     23     2.715856     5.261139    -0.223780
H     24    -2.715856    -5.261139    -0.223780
H     25     2.275588     2.693128    -0.103204
H     26    -2.275588    -2.693128    -0.103204
C     27    -2.898747     2.136884    -0.131985
C     28     2.898747    -2.136884    -0.131985
C     29    -3.280926     2.548417     1.297309
C     30     3.280926    -2.548417     1.297309
C     31    -4.577162     3.368046     1.331643
C     32     4.577162    -3.368046     1.331643
C     33    -4.999676     3.770987     2.750835
C     34     4.999676    -3.770987     2.750835
C     35    -6.295994     4.590889     2.793122
C     36     6.295994    -4.590889     2.793122
C     37    -6.721425     4.993472     4.211309
C     38     6.721425    -4.993472     4.211309
C     39    -8.017746     5.813463     4.255983
C     40     8.017746    -5.813463     4.255983
C     41    -8.435069     6.211453     5.676617
C     42     8.435069    -6.211453     5.676617
H     43    -3.688185     1.511522    -0.555823
H     44     3.688185    -1.511522    -0.555823
H     45    -2.795833     3.005702    -0.786136
H     46     2.795833    -3.005702    -0.786136
H     47    -3.398828     1.639729     1.900389
```

```
H    48     3.398828    -1.639729     1.900389
H    49    -2.465709     3.126630     1.749325
H    50     2.465709    -3.126630     1.749325
H    51    -5.385618     2.788529     0.863670
H    52     5.385618    -2.788529     0.863670
H    53    -4.452648     4.273291     0.720025
H    54     4.452648    -4.273291     0.720025
H    55    -5.123802     2.865006     3.361120
H    56     5.123802    -2.865006     3.361120
H    57    -4.189793     4.348465     3.219331
H    58     4.189793    -4.348465     3.219331
H    59    -7.105001     4.012972     2.323084
H    60     7.105001    -4.012972     2.323084
H    61    -6.171507     5.496815     2.182018
H    62     6.171507    -5.496815     2.182018
H    63    -6.846316     4.087984     4.823082
H    64     6.846316    -4.087984     4.823082
H    65    -5.912724     5.571479     4.682245
H    66     5.912724    -5.571479     4.682245
H    67    -8.826117     5.235997     3.786183
H    68     8.826117    -5.235997     3.786183
H    69    -7.893411     6.718385     3.644925
H    70     7.893411    -6.718385     3.644925
H    71    -8.600230     5.326279     6.302607
H    72     8.600230    -5.326279     6.302607
H    73    -7.660867     6.819137     6.160396
H    74     7.660867    -6.819137     6.160396
H    75    -9.362558     6.794655     5.672987
H    76     9.362558    -6.794655     5.672987
S    77     1.833113     8.065797    -0.314879
C    78    -0.712956     7.771997    -0.658511
C    79    -0.472431     9.164525    -0.712794
C    80     0.859417     9.507347    -0.552141
H    81    -1.253391     9.897200    -0.881281
H    82    -1.698096     7.335429    -0.779563
S    83     0.483578    12.274500    -0.470923
C    84     1.890089    13.316871    -0.527045
C    85     3.037043    12.563046    -0.597832
C    86     2.805858    11.158646    -0.615397
C    87     1.468679    10.819173    -0.555726
H    88     3.600395    10.423256    -0.681349
H    89     4.025343    13.008497    -0.639416
C    90     1.755414    14.813281    -0.518369
C    91     1.178400    15.407915    -1.820700
C    92     1.096099    16.939068    -1.786931
C    93     0.524990    17.545379    -3.075595
C    94     0.439392    19.077319    -3.048071
C    95    -0.132423    19.674851    -4.339038
H    96     1.130221    15.130028     0.327078
H    97     2.753683    15.231049    -0.340455
H    98     0.178083    14.991424    -1.998139
```

```
H      99      1.802706     15.087971     -2.665253
H     100      0.476151     17.250263     -0.933688
H     101      2.098754     17.352338     -1.605218
H     102     -0.477367     17.131264     -3.258002
H     103      1.144973     17.233758     -3.928786
H     104     -0.180161     19.388745     -2.195605
H     105      1.440841     19.491428     -2.866049
H     106     -1.147164     19.305488     -4.530019
H     107      0.485292     19.408858     -5.205224
H     108     -0.180093     20.768122     -4.286915
S     109     -1.833113     -8.065797     -0.314879
C     110      0.712956     -7.771997     -0.658511
C     111      0.472431     -9.164525     -0.712794
C     112     -0.859417     -9.507347     -0.552141
H     113      1.253391     -9.897200     -0.881281
H     114      1.698096     -7.335429     -0.779563
S     115     -0.483578    -12.274500     -0.470923
C     116     -1.890089    -13.316871     -0.527045
C     117     -3.037043    -12.563046     -0.597832
C     118     -2.805858    -11.158646     -0.615397
C     119     -1.468679    -10.819173     -0.555726
H     120     -3.600395    -10.423256     -0.681349
H     121     -4.025343    -13.008497     -0.639416
C     122     -1.755414    -14.813281     -0.518369
C     123     -1.178400    -15.407915     -1.820700
C     124     -1.096099    -16.939068     -1.786931
C     125     -0.524990    -17.545379     -3.075595
C     126     -0.439392    -19.077319     -3.048071
C     127      0.132423    -19.674851     -4.339038
H     128     -1.130221    -15.130028      0.327078
H     129     -2.753683    -15.231049     -0.340455
H     130     -0.178083    -14.991424     -1.998139
H     131     -1.802706    -15.087971     -2.665253
H     132     -0.476151    -17.250263     -0.933688
H     133     -2.098754    -17.352338     -1.605218
H     134      0.477367    -17.131264     -3.258002
H     135     -1.144973    -17.233758     -3.928786
H     136      0.180161    -19.388745     -2.195605
H     137     -1.440841    -19.491428     -2.866049
H     138      1.147164    -19.305488     -4.530019
H     139     -0.485292    -19.408858     -5.205224
H     140      0.180093    -20.768122     -4.286915


T3-A
C       1     -0.420406     -0.572422      0.323075
C       2      0.420406      0.572422      0.323075
C       3     -1.791822     -0.123292      0.269240
C       4      1.791822      0.123292      0.269240
C       5     -0.369117      1.726779      0.243643
C       6      0.369117     -1.726779      0.243643
N       7     -1.702519      1.302929      0.244331
```

N	8	1.702519	-1.302929	0.244331
O	9	-2.870782	-0.727446	0.260186
O	10	2.870782	0.727446	0.260186
C	11	0.099885	3.078641	0.118626
C	12	-0.099885	-3.078641	0.118626
S	13	-0.878663	4.462205	-0.369979
S	14	0.878663	-4.462205	-0.369979
C	15	0.496387	5.545165	-0.306851
C	16	-0.496387	-5.545165	-0.306851
C	17	1.640128	4.849582	0.064553
C	18	-1.640128	-4.849582	0.064553
C	19	1.423402	3.479437	0.294017
C	20	-1.423402	-3.479437	0.294017
C	21	0.350124	6.944387	-0.618515
C	22	-0.350124	-6.944387	-0.618515
H	23	2.609802	5.322286	0.171243
H	24	-2.609802	-5.322286	0.171243
H	25	2.202801	2.776451	0.564050
H	26	-2.202801	-2.776451	0.564050
C	27	-2.918161	2.111235	0.371787
C	28	2.918161	-2.111235	0.371787
C	29	-3.126691	2.758578	1.761864
C	30	3.126691	-2.758578	1.761864
C	31	-4.310458	3.744509	1.670163
C	32	4.310458	-3.744509	1.670163
C	33	-4.559597	4.573635	2.937870
C	34	4.559597	-4.573635	2.937870
C	35	-5.667642	5.621428	2.762347
C	36	5.667642	-5.621428	2.762347
C	37	-5.925050	6.447139	4.028252
C	38	5.925050	-6.447139	4.028252
C	39	-3.258437	1.719054	2.899329
C	40	3.258437	-1.719054	2.899329
C	41	-4.544753	0.880900	2.908747
C	42	4.544753	-0.880900	2.908747
H	43	-3.738295	1.426892	0.143233
H	44	3.738295	-1.426892	0.143233
H	45	-2.924251	2.878023	-0.407704
H	46	2.924251	-2.878023	-0.407704
H	47	-6.718662	7.185480	3.869374
H	48	6.718662	-7.185480	3.869374
H	49	-2.230273	3.352816	1.984977
H	50	2.230273	-3.352816	1.984977
H	51	-5.227536	3.200318	1.404985
H	52	5.227536	-3.200318	1.404985
H	53	-4.118954	4.434781	0.836648
H	54	4.118954	-4.434781	0.836648
H	55	-4.825370	3.913956	3.774260
H	56	4.825370	-3.913956	3.774260
H	57	-3.627365	5.079267	3.229270
H	58	3.627365	-5.079267	3.229270

```
H     59    -6.596160     5.117415     2.460005
H     60     6.596160    -5.117415     2.460005
H     61    -5.401314     6.294044     1.935218
H     62     5.401314    -6.294044     1.935218
H     63    -6.229005     5.805417     4.863923
H     64     6.229005    -5.805417     4.863923
H     65    -5.022802     6.988411     4.337378
H     66     5.022802    -6.988411     4.337378
H     67    -3.170201     2.248774     3.855502
H     68     3.170201    -2.248774     3.855502
H     69    -2.391855     1.047264     2.857495
H     70     2.391855    -1.047264     2.857495
H     71    -5.436638     1.502534     3.042048
H     72     5.436638    -1.502534     3.042048
H     73    -4.661728     0.307450     1.984355
H     74     4.661728    -0.307450     1.984355
H     75    -4.520048     0.164056     3.736807
H     76     4.520048    -0.164056     3.736807
S     77     1.749566     8.010509    -0.654918
C     78    -0.797944     7.656667    -0.922190
C     79    -0.569503     9.030726    -1.166954
C     80     0.759490     9.403378    -1.057869
H     81    -1.361151     9.732969    -1.402129
H     82    -1.782653     7.204096    -0.956791
S     83     0.443820    12.031263    -1.951259
C     84     1.789516    13.141345    -1.794317
C     85     2.867007    12.503830    -1.227442
C     86     2.628312    11.137194    -0.908622
C     87     1.355880    10.709609    -1.232385
H     88     3.368411    10.494039    -0.444965
H     89     3.809887    13.006958    -1.041033
C     90     1.674746    14.575308    -2.227965
C     91     0.759490    15.439887    -1.335011
C     92     0.705933    16.905056    -1.785421
C     93    -0.201133    17.777865    -0.907997
C     94    -0.258680    19.245244    -1.353456
C     95    -1.167463    20.110117    -0.472147
H     96     2.686078    14.999446    -2.228329
H     97     1.315167    14.627086    -3.264318
H     98     1.116462    15.382821    -0.298324
H     99    -0.254526    15.018710    -1.338412
H    100     1.723156    17.322644    -1.783079
H    101     0.356927    16.951816    -2.827155
H    102     0.147461    17.730389     0.133954
H    103    -1.218442    17.360064    -0.909924
H    104     0.757644    19.663099    -1.351145
H    105    -0.606775    19.292791    -2.394656
H    106    -0.824398    20.109949     0.569444
H    107    -2.198531    19.736733    -0.481265
H    108    -1.186582    21.149975    -0.816476
S    109    -1.749566    -8.010509    -0.654918
```

```
C   110    0.797944   -7.656667   -0.922190
C   111    0.569503   -9.030726   -1.166954
C   112   -0.759490   -9.403378   -1.057869
H   113    1.361151   -9.732969   -1.402129
H   114    1.782653   -7.204096   -0.956791
S   115   -0.443820  -12.031263   -1.951259
C   116   -1.789516  -13.141345   -1.794317
C   117   -2.867007  -12.503830   -1.227442
C   118   -2.628312  -11.137194   -0.908622
C   119   -1.355880  -10.709609   -1.232385
H   120   -3.368411  -10.494039   -0.444965
H   121   -3.809887  -13.006958   -1.041033
C   122   -1.674746  -14.575308   -2.227965
C   123   -0.759490  -15.439887   -1.335011
C   124   -0.705933  -16.905056   -1.785421
C   125    0.201133  -17.777865   -0.907997
C   126    0.258680  -19.245244   -1.353456
C   127    1.167463  -20.110117   -0.472147
H   128   -1.315167  -14.627086   -3.264318
H   129   -2.686078  -14.999446   -2.228329
H   130    0.254526  -15.018710   -1.338412
H   131   -1.116462  -15.382821   -0.298324
H   132   -0.356927  -16.951816   -2.827155
H   133   -1.723156  -17.322644   -1.783079
H   134    1.218442  -17.360064   -0.909924
H   135   -0.147461  -17.730389    0.133954
H   136    0.606775  -19.292791   -2.394656
H   137   -0.757644  -19.663099   -1.351145
H   138    2.198531  -19.736733   -0.481265
H   139    0.824398  -20.109949    0.569444
H   140    1.186582  -21.149975   -0.816476
```

5. Calculated absorption spectra of all molecules in chlorobenzene

a) Transitions calculated by PCM/TD CAM-B3LYP/6-31++G(d,p) method

T1-B

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
1	2.4498	506.09	0.7081
2	3.5100	353.23	0.0001
3	3.9543	313.54	0.0003
4	4.1698	297.34	0.0000
5	4.3048	288.02	0.5687
6	4.4362	279.48	0.0012
7	4.5319	273.58	0.0174
8	4.6315	267.70	0.1128
9	4.6447	266.94	0.0000
10	4.9229	251.85	0.0003
11	4.9961	248.16	0.1983
12	5.3889	230.07	0.0010
13	5.5383	223.87	0.0000

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
14	5.5512	223.35	0.0000
15	5.6708	218.63	0.0022
16	5.6960	217.67	0.0453
17	5.7378	216.08	0.0039
18	5.7684	214.94	0.2697
19	5.8994	210.16	0.0012
20	5.9825	207.25	0.0007
21	6.0369	205.38	0.0002
22	6.0969	203.36	0.0026
23	6.1405	201.91	0.0043
24	6.1473	201.69	0.0005
25	6.1932	200.19	0.0889
26	6.2118	199.59	0.0028
27	6.2351	198.85	0.0090
28	6.2735	197.63	0.0027
29	6.2916	197.06	0.0016
30	6.3817	194.28	0.0001
31	6.3877	194.10	0.0456
32	6.3946	193.89	0.0003
33	6.4013	193.69	0.0042
34	6.4798	191.34	0.0006
35	6.4865	191.14	0.0006
36	6.5354	189.71	0.0000
37	6.5366	189.68	0.0014
38	6.5401	189.58	0.0058
39	6.5486	189.33	0.0187
40	6.5568	189.09	0.0240

T1-A

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
1	2.4819	499.56	0.7010
2	3.5309	351.14	0.0000
3	3.9699	312.31	0.0070
4	4.1420	299.33	0.0000
5	4.2572	291.23	0.4877
6	4.4039	281.53	0.0108
7	4.5109	274.86	0.0447
8	4.6514	266.55	0.0015
9	4.6575	266.21	0.1111
10	4.9512	250.41	0.0175
11	5.0110	247.42	0.1719
12	5.3991	229.64	0.0002
13	5.4944	225.66	0.0027
14	5.5670	222.71	0.0002
15	5.6493	219.47	0.0369
16	5.7069	217.25	0.0039
17	5.7483	215.69	0.2838
18	5.7729	214.77	0.0044
19	5.9013	210.10	0.0047
20	5.9795	207.35	0.0010
21	6.0479	205.00	0.0057

22	6.0946	203.43	0.0004
23	6.1027	203.16	0.0019
24	6.1225	202.51	0.0520
25	6.1356	202.07	0.0019
26	6.1934	200.19	0.0346
27	6.2162	199.45	0.0065
28	6.2628	197.97	0.0027
29	6.3199	196.18	0.0048
30	6.3747	194.49	0.0291
31	6.3751	194.48	0.0019
32	6.3785	194.38	0.0016
33	6.3793	194.35	0.0000
34	6.3858	194.16	0.0456
35	6.4067	193.52	0.0000
36	6.4743	191.50	0.0083
37	6.4764	191.44	0.0003
38	6.4863	191.15	0.0000
39	6.5388	189.61	0.0000
40	6.5473	189.37	0.0198

T2-B

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
1	2.0936	592.21	1.6136
2	3.1838	389.43	0.0116
3	3.5020	354.04	0.0004
4	3.5137	352.86	0.8281
5	3.5800	346.32	0.0010
6	4.1040	302.10	0.0746
7	4.1544	298.44	0.0000
8	4.4232	280.30	0.0007
9	4.4833	276.54	0.0392
10	4.5082	275.02	0.0097
11	4.5766	270.91	0.0027
12	4.7390	261.63	0.0003
13	4.7827	259.24	0.0039
14	4.8164	257.42	0.0006
15	4.8214	257.15	0.1976
16	5.0387	246.06	0.0001
17	5.0681	244.64	0.0004
18	5.0856	243.79	0.0218
19	5.1588	240.34	0.0005
20	5.2247	237.31	0.0016
21	5.2548	235.94	0.0000
22	5.3004	233.92	0.0000
23	5.3402	232.17	0.0003
24	5.3653	231.08	0.0002
25	5.3985	229.66	0.0015
26	5.4161	228.92	0.0101
27	5.4715	226.60	0.1193
28	5.5353	223.99	0.0000
29	5.5445	223.62	0.0734

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
30	5.6622	218.97	0.0037
31	5.6726	218.57	0.0034
32	5.6847	218.10	0.0001
33	5.7479	215.70	0.0006
34	5.7680	214.95	0.0002
35	5.8127	213.30	0.0019
36	5.8228	212.93	0.0010
37	5.8300	212.66	0.0003
38	5.8319	212.60	0.0514
39	5.8939	210.36	0.0006
40	5.9392	208.75	0.0294

T2-A

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
1	2.1246	583.57	1.5790
2	3.1984	387.65	0.0492
3	3.5177	352.46	0.0013
4	3.5186	352.36	0.7898
5	3.6005	344.36	0.0014
6	4.1161	301.22	0.0861
7	4.1317	300.08	0.0003
8	4.4218	280.39	0.0000
9	4.4546	278.33	0.0350
10	4.5244	274.04	0.0087
11	4.5789	270.77	0.0086
12	4.7648	260.21	0.0038
13	4.7927	258.69	0.0021
14	4.8258	256.92	0.0011
15	4.8331	256.53	0.1863
16	5.0386	246.07	0.0000
17	5.0670	244.69	0.0186
18	5.0837	243.88	0.0000
19	5.1682	239.90	0.0004
20	5.2101	237.97	0.0017
21	5.2316	236.99	0.0005
22	5.2982	234.01	0.0001
23	5.3164	233.21	0.0000
24	5.3659	231.06	0.0134
25	5.4061	229.34	0.0310
26	5.4080	229.26	0.0011
27	5.4649	226.87	0.0782
28	5.5325	224.10	0.1120
29	5.5408	223.77	0.0009
30	5.6537	219.30	0.0036
31	5.6663	218.81	0.0029
32	5.6776	218.37	0.0025
33	5.7466	215.75	0.0000
34	5.7882	214.20	0.0001
35	5.8148	213.22	0.0418
36	5.8240	212.88	0.0000
37	5.8442	212.15	0.0014

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
38	5.8527	211.84	0.0025
39	5.9016	210.09	0.0000
40	5.9304	209.06	0.0189

T2-D

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
1	2.2184	558.90	1.3497
2	3.4107	363.52	0.0119
3	3.5358	350.65	0.0035
4	3.6722	337.63	0.6817
5	3.7603	329.72	0.0007
6	4.1544	298.44	0.0000
7	4.3381	285.80	0.1085
8	4.4869	276.32	0.0230
9	4.5280	273.81	0.0000
10	4.5739	271.07	0.0653
11	4.6987	263.87	0.0278
12	4.6992	263.84	0.1198
13	4.7093	263.27	0.0102
14	4.8159	257.45	0.0001
15	4.9586	250.04	0.0860
16	5.1128	242.50	0.0032
17	5.1460	240.93	0.0630
18	5.2418	236.53	0.0004
19	5.2874	234.49	0.0024
20	5.3452	231.95	0.0041
21	5.4105	229.16	0.0265
22	5.4209	228.72	0.0003
23	5.4523	227.40	0.0000
24	5.4688	226.71	0.0001
25	5.5146	224.83	0.0021
26	5.5259	224.37	0.0695
27	5.5917	221.73	0.0928
28	5.6220	220.53	0.0015
29	5.6516	219.38	0.1335
30	5.7221	216.68	0.0329
31	5.7352	216.18	0.0414
32	5.7658	215.03	0.0037
33	5.7910	214.10	0.0305
34	5.8071	213.50	0.0009
35	5.8498	211.95	0.0120
36	5.8842	210.71	0.0101
37	5.9077	209.87	0.0104
38	5.9387	208.77	0.0020
39	5.9834	207.21	0.0227
40	5.9868	207.10	0.0002

T2-C

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
1	2.2510	550.78	1.3004
2	3.4183	362.70	0.0497

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
3	3.5468	349.56	0.0115
4	3.6630	338.48	0.6249
5	3.7773	328.24	0.0006
6	4.1256	300.53	0.0002
7	4.3381	285.81	0.1196
8	4.4633	277.78	0.0320
9	4.5239	274.07	0.0000
10	4.5802	270.69	0.0475
11	4.6989	263.86	0.0068
12	4.7163	262.88	0.1089
13	4.7174	262.82	0.0487
14	4.8486	255.71	0.0006
15	4.9540	250.27	0.0794
16	5.1035	242.94	0.0046
17	5.1454	240.96	0.0624
18	5.2572	235.84	0.0005
19	5.3000	233.93	0.0022
20	5.3321	232.52	0.0082
21	5.4086	229.23	0.0310
22	5.4327	228.22	0.0000
23	5.4488	227.54	0.0000
24	5.4530	227.37	0.0007
25	5.5258	224.38	0.0889
26	5.5377	223.89	0.0019
27	5.5992	221.43	0.0975
28	5.6186	220.67	0.0001
29	5.6434	219.70	0.1178
30	5.7213	216.70	0.0569
31	5.7284	216.44	0.0253
32	5.7507	215.60	0.0039
33	5.7910	214.10	0.0171
34	5.8359	212.45	0.0151
35	5.8403	212.29	0.0068
36	5.8863	210.63	0.0012
37	5.9143	209.63	0.0422
38	5.9631	207.92	0.0033
39	5.9714	207.63	0.0367
40	5.9719	207.61	0.0059

T3-B

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
1	1.9813	625.77	2.2115
2	2.8411	436.39	0.0087
3	3.1584	392.56	1.0635
4	3.3351	371.76	0.0000
5	3.4966	354.58	0.0003
6	3.7151	333.73	0.0685
7	3.8976	318.10	0.0000
8	4.1365	299.73	0.0000
9	4.2028	295.01	0.0284
10	4.4092	281.20	0.0526

11	4.4560	278.24	0.0000
12	4.4574	278.15	0.0288
13	4.4649	277.69	0.0001
14	4.4977	275.66	0.0140
15	4.5646	271.62	0.0626
16	4.6484	266.72	0.0007
17	4.7036	263.60	0.0012
18	4.7234	262.49	0.0002
19	4.7527	260.87	0.0520
20	4.8348	256.44	0.0018
21	4.9279	251.60	0.0001
22	4.9695	249.49	0.1605
23	4.9746	249.23	0.0000
24	5.0217	246.90	0.0025
25	5.0973	243.23	0.0000
26	5.1154	242.38	0.0056
27	5.1450	240.98	0.0000
28	5.1626	240.16	0.2312
29	5.2317	236.99	0.0003
30	5.2411	236.56	0.0145
31	5.3133	233.35	0.0350
32	5.3200	233.05	0.0000
33	5.3304	232.60	0.0018
34	5.3422	232.08	0.0043
35	5.3657	231.07	0.0031
36	5.4348	228.13	0.0612
37	5.4446	227.72	0.0000
38	5.4704	226.65	0.0854
39	5.5013	225.37	0.0246
40	5.5620	222.91	0.0201

T3-A

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
1	2.0044	618.57	2.1705
2	2.8426	436.17	0.0789
3	3.1628	392.00	1.0197
4	3.3480	370.32	0.0005
5	3.5137	352.86	0.0008
6	3.7157	333.68	0.0732
7	3.8943	318.38	0.0014
8	4.1128	301.46	0.0001
9	4.2035	294.96	0.0284
10	4.3952	282.09	0.0406
11	4.4250	280.19	0.0359
12	4.4479	278.75	0.0065
13	4.4686	277.46	0.0000
14	4.5124	274.76	0.0170
15	4.5670	271.48	0.0489
16	4.6461	266.86	0.0001
17	4.7074	263.38	0.0001
18	4.7459	261.25	0.0090

19	4.7583	260.56	0.0449
20	4.8263	256.89	0.0002
21	4.9345	251.26	0.0002
22	4.9749	249.22	0.1426
23	4.9792	249.00	0.0160
24	5.0255	246.71	0.0003
25	5.0840	243.87	0.0000
26	5.1194	242.18	0.0002
27	5.1574	240.40	0.0000
28	5.1579	240.38	0.2207
29	5.2248	237.30	0.0002
30	5.2506	236.14	0.0152
31	5.2988	233.99	0.0006
32	5.3055	233.69	0.0603
33	5.3370	232.31	0.0034
34	5.3388	232.23	0.0008
35	5.3860	230.20	0.0013
36	5.4043	229.42	0.0676
37	5.4248	228.55	0.0001
38	5.4559	227.25	0.0767
39	5.5205	224.59	0.0102
40	5.5321	224.12	0.0592

b) Transitions calculated by PCM/TD PBE0/6-31++G(d,p) method

T1-B

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
1	2.3121	536.25	0.6662
2	3.2506	381.42	0.0002
3	3.5424	350.00	0.0000
4	3.7235	332.98	0.0000
5	3.8441	322.53	0.4139
6	4.0195	308.46	0.0010
7	4.0767	304.13	0.0086
8	4.1127	301.47	0.0502
9	4.1339	299.92	0.0002
10	4.5492	272.54	0.3028
11	4.7888	258.90	0.0000
12	4.9164	252.18	0.0005
13	5.0217	246.90	0.0002
14	5.0484	245.59	0.0000
15	5.1210	242.11	0.1788
16	5.2375	236.72	0.0006
17	5.2549	235.94	0.0002
18	5.3380	232.26	0.0015
19	5.3526	231.63	0.0003
20	5.3755	230.65	0.0029
21	5.3797	230.47	0.0252
22	5.4201	228.75	0.0073
23	5.4334	228.19	0.0002
24	5.4511	227.45	0.0638

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
25	5.4866	225.98	0.0020
26	5.5122	224.93	0.0004
27	5.5686	222.65	0.0002
28	5.5903	221.78	0.0001
29	5.5938	221.65	0.0387
30	5.6096	221.02	0.0094
31	5.6284	220.28	0.0001
32	5.6313	220.17	0.0006
33	5.6710	218.63	0.0138
34	5.6996	217.53	0.0015
35	5.7053	217.31	0.0008
36	5.7177	216.84	0.0010
37	5.7410	215.96	0.0000
38	5.7752	214.68	0.0010
39	5.7785	214.56	0.0000
40	5.8302	212.66	0.0015

T1-A

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
1	2.3371	530.50	0.6555
2	3.2567	380.71	0.0004
3	3.5579	348.48	0.0005
4	3.6894	336.05	0.0002
5	3.7954	326.67	0.3639
6	3.9799	311.52	0.0144
7	4.0381	307.03	0.0248
8	4.1370	299.70	0.0002
9	4.1455	299.08	0.0518
10	4.5484	272.59	0.2741
11	4.7626	260.33	0.0048
12	4.9049	252.78	0.0001
13	5.0267	246.65	0.0001
14	5.0313	246.43	0.0010
15	5.0957	243.31	0.1700
16	5.2116	237.90	0.0007
17	5.2301	237.06	0.0001
18	5.2749	235.05	0.0003
19	5.2858	234.56	0.0000
20	5.3126	233.38	0.0085
21	5.3274	232.73	0.0056
22	5.3329	232.49	0.0079
23	5.3561	231.48	0.0024
24	5.3753	230.65	0.0321
25	5.4117	229.10	0.0000
26	5.4227	228.64	0.0424
27	5.4418	227.84	0.0296
28	5.4843	226.07	0.0002
29	5.5002	225.42	0.0032
30	5.5164	224.76	0.0018
31	5.5739	222.44	0.0038
32	5.5830	222.07	0.0037

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
33	5.6068	221.13	0.0468
34	5.6756	218.45	0.0013
35	5.7153	216.94	0.0031
36	5.7355	216.17	0.0000
37	5.7598	215.26	0.0001
38	5.7790	214.54	0.0000
39	5.8037	213.63	0.0165
40	5.8790	210.89	0.0009

T2-B

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
1	1.8976	653.38	1.6819
2	2.7664	448.19	0.0005
3	2.9661	418.01	0.0124
4	3.0219	410.29	0.3946
5	3.2095	386.30	0.0001
6	3.5598	348.29	0.3212
7	3.6753	337.35	0.0000
8	3.8994	317.96	0.2068
9	3.9214	316.17	0.0000
10	3.9300	315.48	0.0068
11	4.0208	308.36	0.0008
12	4.0926	302.95	0.0000
13	4.1119	301.53	0.0026
14	4.1345	299.88	0.0571
15	4.1764	296.87	0.0014
16	4.3602	284.35	0.0236
17	4.5496	272.52	0.0001
18	4.5559	272.14	0.0000
19	4.5963	269.75	0.0229
20	4.6085	269.03	0.0013
21	4.6149	268.66	0.0005
22	4.6931	264.18	0.0015
23	4.7822	259.26	0.0000
24	4.7909	258.79	0.0120
25	4.8190	257.28	0.0043
26	4.8273	256.84	0.0001
27	4.8513	255.57	0.0657
28	4.9468	250.64	0.0002
29	4.9712	249.40	0.0001
30	4.9917	248.38	0.0001
31	5.0126	247.35	0.0005
32	5.0374	246.13	0.0017
33	5.0453	245.74	0.0037
34	5.0602	245.02	0.0004
35	5.1238	241.98	0.0013
36	5.1308	241.65	0.0172
37	5.1880	238.98	0.0000
38	5.1930	238.75	0.0065
39	5.2041	238.24	0.1076
40	5.2060	238.16	0.0000

T2-A

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
1	1.9213	645.30	1.6391
2	2.7791	446.14	0.0027
3	2.9780	416.33	0.0472
4	3.0248	409.89	0.3729
5	3.2135	385.83	0.0000
6	3.5790	346.42	0.3175
7	3.6504	339.64	0.0003
8	3.9002	317.89	0.2067
9	3.9260	315.80	0.0066
10	3.9280	315.64	0.0014
11	4.0072	309.40	0.0077
12	4.0933	302.89	0.0001
13	4.1163	301.20	0.0036
14	4.1220	300.79	0.0438
15	4.1665	297.57	0.0050
16	4.3390	285.75	0.0204
17	4.5230	274.12	0.0007
18	4.5349	273.40	0.0002
19	4.5925	269.97	0.0258
20	4.5926	269.96	0.0010
21	4.6295	267.82	0.0000
22	4.6783	265.02	0.0045
23	4.7569	260.64	0.0000
24	4.7585	260.55	0.0061
25	4.8130	257.60	0.0000
26	4.8323	256.57	0.0499
27	4.8777	254.18	0.0248
28	4.9191	252.05	0.0002
29	4.9699	249.47	0.0003
30	5.0001	247.96	0.0004
31	5.0074	247.60	0.0085
32	5.0348	246.25	0.0006
33	5.0612	244.97	0.0008
34	5.0695	244.57	0.0001
35	5.0978	243.21	0.0239
36	5.1302	241.68	0.0011
37	5.1855	239.10	0.0034
38	5.1855	239.10	0.0003
39	5.1893	238.92	0.0349
40	5.1934	238.73	0.0000

T2-D

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
1	2.0297	610.85	1.3842
2	2.9718	417.21	0.0019
3	3.1400	394.85	0.3284
4	3.1542	393.08	0.0123
5	3.2373	382.99	0.0005

6	3.6860	336.36	0.0001
7	3.7562	330.08	0.2011
8	3.8102	325.40	0.0712
9	3.8116	325.28	0.0060
10	4.0130	308.96	0.0098
11	4.0451	306.51	0.0006
12	4.0751	304.25	0.0411
13	4.1908	295.85	0.0010
14	4.2061	294.77	0.1826
15	4.3361	285.93	0.0522
16	4.3535	284.79	0.0043
17	4.5228	274.13	0.0010
18	4.6288	267.86	0.0046
19	4.7084	263.32	0.0211
20	4.7608	260.43	0.0001
21	4.8030	258.14	0.0557
22	4.8374	256.30	0.0169
23	4.8662	254.79	0.0005
24	4.8879	253.66	0.0005
25	4.9009	252.98	0.0002
26	4.9646	249.74	0.0633
27	4.9728	249.33	0.0250
28	4.9793	249.00	0.0075
29	4.9896	248.48	0.0289
30	5.0127	247.34	0.0015
31	5.0432	245.84	0.0506
32	5.0854	243.80	0.0004
33	5.1419	241.12	0.0323
34	5.1588	240.34	0.0061
35	5.1683	239.89	0.0005
36	5.2090	238.02	0.0026
37	5.2556	235.91	0.0056
38	5.2759	235.00	0.0006
39	5.2781	234.90	0.0287
40	5.2994	233.96	0.0954

T2-C

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
1	2.0556	603.15	1.3256
2	2.9704	417.39	0.0100
3	3.1281	396.36	0.2938
4	3.1650	391.73	0.0410
5	3.2402	382.64	0.0047
6	3.6540	339.31	0.0000
7	3.7644	329.36	0.1877
8	3.8156	324.94	0.0745
9	3.8177	324.76	0.0051
10	3.9858	311.06	0.0137
11	4.0387	306.99	0.0023
12	4.0638	305.09	0.0335
13	4.1874	296.09	0.0034

14	4.1990	295.27	0.1815
15	4.3261	286.60	0.0503
16	4.3453	285.33	0.0138
17	4.5031	275.33	0.0012
18	4.6142	268.70	0.0024
19	4.7179	262.80	0.0260
20	4.7810	259.33	0.0001
21	4.8081	257.86	0.0612
22	4.8448	255.91	0.0079
23	4.8452	255.89	0.0038
24	4.8909	253.50	0.0008
25	4.9100	252.52	0.0005
26	4.9613	249.90	0.0519
27	4.9717	249.38	0.0256
28	4.9771	249.11	0.0241
29	4.9916	248.39	0.0079
30	5.0036	247.79	0.0339
31	5.0234	246.81	0.0385
32	5.0994	243.13	0.0000
33	5.1184	242.23	0.0106
34	5.1494	240.78	0.0262
35	5.1715	239.75	0.0010
36	5.2090	238.02	0.0007
37	5.2110	237.93	0.0000
38	5.2117	237.90	0.0042
39	5.2631	235.57	0.0002
40	5.2748	235.05	0.0062

T3-B

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
1	1.7317	715.98	2.3823
2	2.3934	518.02	0.0024
3	2.6023	476.44	0.0061
4	2.6572	466.59	0.2405
5	3.0960	400.46	0.4500
6	3.1773	390.21	0.0001
7	3.2726	378.85	0.3609
8	3.5141	352.82	0.0011
9	3.5655	347.73	0.0000
10	3.6356	341.03	0.0776
11	3.6450	340.15	0.0000
12	3.7346	331.99	0.0001
13	3.7923	326.93	0.0001
14	3.9077	317.28	0.0148
15	3.9300	315.48	0.0001
16	3.9903	310.71	0.0068
17	4.0073	309.39	0.0002
18	4.0086	309.29	0.0066
19	4.0375	307.08	0.0437
20	4.0872	303.35	0.0274
21	4.1738	297.06	0.0003

22	4.2009	295.14	0.0378
23	4.3236	286.76	0.0532
24	4.4078	281.28	0.0001
25	4.4396	279.27	0.0336
26	4.5038	275.29	0.0001
27	4.5318	273.59	0.0000
28	4.5494	272.53	0.0003
29	4.5646	271.62	0.0098
30	4.5968	269.72	0.0002
31	4.6258	268.03	0.0063
32	4.6561	266.28	0.0019
33	4.6588	266.13	0.0004
34	4.7327	261.97	0.0028
35	4.7383	261.67	0.0011
36	4.7448	261.30	0.0193
37	4.7477	261.15	0.0003
38	4.7939	258.63	0.0134
39	4.8049	258.04	0.0001
40	4.8225	257.09	0.0000

T3-A

No.	Energy [eV]	Wavelength [nm]	Oscill.strength
1	1.7471	709.66	2.3212
2	2.3938	517.93	0.0210
3	2.6119	474.70	0.0548
4	2.6643	465.35	0.2224
5	3.1050	399.30	0.4642
6	3.1798	389.91	0.0000
7	3.2662	379.60	0.3420
8	3.5140	352.83	0.0096
9	3.5710	347.20	0.0001
10	3.6151	342.96	0.0002
11	3.6180	342.69	0.0644
12	3.7295	332.44	0.0017
13	3.7827	327.76	0.0014
14	3.8990	317.99	0.0178
15	3.9357	315.02	0.0018
16	3.9782	311.66	0.0092
17	4.0068	309.44	0.0000
18	4.0161	308.72	0.0019
19	4.0362	307.18	0.0463
20	4.0895	303.18	0.0237
21	4.1756	296.92	0.0018
22	4.1994	295.24	0.0332
23	4.3163	287.25	0.0536
24	4.3893	282.47	0.0000
25	4.4248	280.20	0.0378
26	4.4777	276.89	0.0006
27	4.5192	274.35	0.0006
28	4.5488	272.57	0.0101
29	4.5523	272.36	0.0004

```
30        4.6001        269.52        0.0004
31        4.6201        268.36        0.0014
32        4.6667        265.68        0.0016
33        4.6799        264.93        0.0004
34        4.7108        263.19        0.0004
35        4.7139        263.02        0.0035
36        4.7373        261.72        0.0015
37        4.7396        261.59        0.0159
38        4.7836        259.18        0.0119
39        4.7989        258.36        0.0010
40        4.8136        257.57        0.0005
```

References

[1] L. Dou, J. Gao, E. Richard,J. You, C-C. Chen, K. C. Cha, Y. He, G. Li, Y Yang, "Systematic investigation of benzodithiophene- and diketopyrrolopyrrole-based low-bandgap polymers designed for single junction and tandem polymer solar cells", *J. Am. Chem. Soc.* 134 (2012) 10071-10079.

[2] S. P. Mishra, A. K. Palai, M. Patri, "Synthesis and characterization of soluble narrow band gap conducting polymers based on diketopyrrolopyrrole and propylenedioxythiophenes", *Synthetic Metals* 160 (2010) 2422–2429.

[3] J. Zhang, D-Y. Kang, S. Barlow, S. R. Marder, "Transition metal-catalyzed C–H activation as a route to structurally diverse di(arylthiophenyl)-diketopyrrolopyrroles", *J. Mater. Chem.*, 22 (2012) 21392-21394.

[4] B. P. Karsten, J. C. Bijleveld, R. A. J. Janssen, "Diketopyrrolopyrroles as Acceptor Materials in Organic Photovoltaics", *Macromol. Rapid. Commun.*, 31 (2010), 1554-1559.

[5] T. Harschneck, N. Zhou, E. F. Manley, S. J. Lou, X. Yu, M. R. Butler, A. Timalsina, R. Turrisi, M. A. Ratner, L. X. Chen, R. P. H. Chang, A. Facchetti, T. J. Marks, "Substantial photovoltaic response and morphology tuning in benzo[1,2-b:6,5-b0]-dithiophene (bBDT) molecular donors, *Chem. Commun.,* 50 (2014) 4099-4101.

[6] C-W. Ge, C-Y. Mei, J. Ling, F-G. Zhao, H-J. Li, L. Liang, J-T. Wang, J-C. Yu, W Shao, Y-S. Xie, W-S. Li, "Diketopyrrolopyrrole-based acceptor–acceptor conjugated polymers: the importance of comonomer on their charge transportation nature", Journal of Polymer Science, Part A: POLYMER CHEMISTRY, 52 (2014) 2356–2366.

[7] S. Stas, S. Sergeyev, Y. Geerts, "Synthesis of diketopyrrolopyrrole (DPP) derivatives comprising bithiophene moieties", *Tetrahedron* 66 (2010) 1837-1845.

[8] C. H. Woo, P. M. Beaujuge, T. W. Holcombe; O. P. Lee, J. M. J. Frechet, "Incorporation of furan into low band-gap polymers for efficient solar cells", *Journal of the American Chemical Society*, 132 (2010) 15547 – 15549.

[9] V. S. Gevaerts, E. M. Herzig, M. Kirkus, K. H. Hendriks, M. M. Wienk, J. Perlich, P. Mu, R. A. J. Janssen, "Influence of the position of the side chain on crystallization and solar cell performance of DPP-based small molecules", *Chem. Mater.*, 26 (2014), 916-926.

[10] A. B. Tamayo, X-D. Dang, B. Walker, J. Seo, T. Kent, T-Q. Nguyena, "A low band gap, solution processable oligothiophene with a dialkylated diketopyrrolopyrrole chromophore for use in bulk heterojunction solar cells", *Appl. Phys. Lett.* 94 (2009) 103301.