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Supporting Information

Tuning the Electronic Properties of p-Conjugated Oligothiophenes with the 3,4-Ethylenedioxythiophene (EDOT) Building Block

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Synthesis and Characterization of all compounds

3,4-Ethylenedioxy-2,2'-bithiophene (2a) :
Preparation of the stannic derivative **1b**: To a solution containing EDOT **1** dissolved in dry THF and under inert atmosphere (N_2), an equivalent of n-BuLi (2,5 M or 1,6 M in hexane) was added dropwise. The mixture was stirred during 1h at the addition temperature. Then, tributyltin chloride was added dropwise and the mixture was stirred at the same temperature during 1/2h before allowing to warm at room temperature. After dilution with diethyl ether, the organic phase was successively washed by a saturated solution of $NaHCO_3$ then with water. After drying on $MgSO_4$, the solvent was evaporated and **1b** was used without other purification in the Stille coupling reactions.
The stannic derivative **1b** (7.05mmol, 1.5 equivalent), 2-bromothiophene (4.7 mmol) and $Pd(PPh_3)_4$ (400mg) were refluxed of anhydrous toluene (50 mL) during 12h, under inert atmosphere (N_2). After concentration, the residue was dissolved in CH_2Cl_2. The organic phase was washed 2 times with a saturated solution of $NaHCO_3$ then with water. After drying on $MgSO_4$ and evaporation of solvent, the product was purified by chromatography on silica gel (CH_2Cl_2 / EP 1/1) to give **2a** as colourless oil (770mg, 73%).
2a: ^{1}H NMR ($CDCl_3$): δ= 4.24 (m, 2H), 4.33 (m, 2H), 6.21 (s, 1H), 7.01 (dd, ^{3}J = 5.1 Hz, ^{3}J = 3.7 Hz), 7.2 (d, ^{3}J = 5.1 Hz, 1H,), 7.22 (d, ^{3}J = 3.7 Hz, 1H); elemental analysis calculated (%) for $C_{10}H_8O_2S_2$: C 53.55, H 3.60, O 14.27, S 28.59; found: C 53.82, H 3.49, O 14.47, S 27.89.

3,4-Ethylenedioxy-5'-hexyl-2,2'-bithiophene (3a) : Analogously to **2a** in toluene (50mL) by using 2-bromo-5-hexylthiophene (900mg, 3.64mmol), **1b** (5.28mmol, 1.5 eq) and $Pd(PPh_3)_4$ (300mg). The product was purified by chromatography on silica gel (CH_2Cl_2 / EP 3/1) to obtain **3a** as orange oil (550mg, 49%).
3a: ^{1}H NMR ($CDCl_3$): δ= 0.9 (t, ^{3}J = 6.8 Hz, 3H), 1.34 (m, 6H), 1.67 (m, 2H), 2.79 (t, ^{3}J = 7.6 Hz, 2H), 4.24 (m, 2H), 4.32 (m, 2H), 6.17 (s, 1H), 6.67 (d, ^{3}J = 3.5 Hz, 1H), 7.02 (d, ^{3}J = 3.5 Hz, 1H); HRMS calculated for $C_{16}H_{20}O_2S_2$: 308.0905; found: 308.0919.

3',4'-Ethylenedioxy-2,2':5',2''terthiophene (4a) :

The distannic derivative **1c** was prepared by the same procedure described for **1b** starting from EDOT **1** and two equivalent of n-BuLi and a slight excess of $ClSnBu_3$**.** The product was used without other purification for the Stille coupling reaction.
The Stille coupling was done according to the procedure described for **2a** in toluene (50mL) by using 2-bromothiophene (2.5g, 15.5mmol), **1c** (7.04mmol) and $Pd(PPh_3)_4$ (800mg). The product was purified by chromatography on silica gel (CH_2Cl_2 / EP 1/1) to obtain **4a** as orange solide (720mg, 33%).

4a: M.p.= 125°C; ^{1}H NMR ($CDCl_3$): δ = 4.4 (s, 4H), 7.03 (m, 2H), 7.23 (m,4H); ^{13}C NMR ($CDCl_3$): δ = 137.43, 134.36, 127.16, 123.90, 122.86, 109.46, 64.92; MS (MALDI-TOF) calculated for $C_{14}H_{10}O_2S_3$: 305.98; found: 306.11.

5,5''-Dibromo-3',4'-éthylènedioxy-2,2':5',2''terthiophène (4b) : NBS (3.73g, 20.8mmol) was added by portion to a solution of **4a** (3.2g, 10.4mmol) in $CHCl_3$ (50mL) at -20°C and under inert atmosphere (N_2), The mixture was stirred during 2h at the addition temperature then 1h at room temperature. The solution was concentrated and the residue was dissolved in CH_2Cl_2. After washing with water, the organic phase was dried on $MgSO_4$ and then concentrated. The product was recrystallized from a $CHCl_3$ / absolute ethanol mixture to give **4b** as orange solid (4g, 82%).
4b: M.p.=195°C; ^{1}H NMR ($CDCl_3$): δ = 4.38 (s, 4H), 6.92 (d, ^{3}J = 3.9 Hz, 2H), 6.96 (d, ^{3}J = 3.9 Hz, 2H); ^{13}C NMR (500MHz, $CDCl_3$): δ = 65.00, 109.02, 111.13, 122.59, 129.81, 135.67, 137.61; MS (MALDI-TOF) calculated for $C_{14}H_8Br_2O_2S_3$: 463.85; found: 463.81.

5-Hexyl-2,2'-bis(3,4-ethylenedioxythiophene) (6a) : A solution of bis-EDOT **5a**[16a] in dry THF was cooled to -78°C and n-BuLi (2.5M in hexane, 1.42mL, 3.54mmol) was added dropwise. The mixture was stirred for 0.5 h (1g, 3.54mmol) and bromohexane (600µL, 4.25mmol) was added. The solution was allowed to warm at room temperature and stirring overnight. After dilution with diethyl ether, the organic phase was successively washed with saturated aqueous NH_4Cl solution and water. The organic phase was dried over $MgSO_4$ and the solvent was evaporated. The product was purified by chromatography on silica gel (CH_2Cl_2 / Petroleum Ether 1/1) to give **6a** (430mg, 27%) and the disubstituted compound (310mg, 25%).
6a : White solid, M.p.= 120°C; ^{1}H NMR ($CDCl_3$): δ = 0.88 (t, ^{3}J = 6.6 Hz, 3H), 1.31 (m, 6H), 1.60 (m, 2H), 2.64 (t, ^{3}J = 7.5 Hz, 2H), 4,23 (m, 4H), 4,30 (m, 4H), 6 ,22 (s, 1H); HRMS calculated for $C_{18}H_{22}O_4S_2$: 366.0960; found : 366.0947.

2-n-Hexyl-3,4-ethylenedioxythiophene (7a) : To a solution of 10g of EDOT **1** (70.4mmol) in dry THF cooled to -78°C 29ml n-BuLi (2.5M in hexane, 74mmol) was added dropwise. The mixture was stirred for 1h, and 15 mL of 1-bromohexane (105,6mmol) was added. The mixture was allowed to warm slowly at room temperature and stirred for an additional 12h. After dilution with diethyl ether, the organic phase was washed successively by a saturated solution of NH_4Cl and then water. After drying over $MgSO_4$ and evaporation of solvent, the residue was distillate with a Kugelrhor apparatus allowing to separate compound **6a** (160°C, 2 mbar) from EDOT (88°C, 8mbar).

7a: colourless oil (6.36g, 40%). ^{1}H NMR ($CDCl_3$): δ = 0.89 (t, ^{3}J = 6.8 Hz, 3H), 1.32-1.39 (m, 6H), 1.40 (m, 2H), 1.55-1.65 (m, 2H) 2.63 (t, ^{3}J = 7.7 Hz, 2H), 4,17 (s, 4H), 6,11 (s, 1H); ^{13}C NMR ($CDCl_3$): δ = 141.38, 137.29, 118.43, 94.95, 64.69, 64.53, 31.55, 30.43, 28.84, 25.94, 22.59, 14.09 ; MS (EI): m/z (%): 226 (100) [$M^{+\cdot}$].

3,4,3"',4"'-Bis(ethylenedioxy)-5,5'''-dihexyl-2,2':5',2":5",2"'-quaterthiophene (ETTE):
The stannic derivative **7b** was prepared by the same procedure described for **1b** starting from **7a**. The product was used without other purification for the Stille coupling reaction.
The Stille coupling was done according to the procedure described for **2a** in toluene (50mL) by using 5,5'-dibromo-2,2'-bithiophene (860mg, 2.65mmol), **7b** (6.62mmol, 2.5 eq) and $Pd(PPh_3)_4$ (300mg). The product was purified by chromatography on silica gel (CH_2Cl_2 / EP 1/1) to give **ETTE** as orange solid (920mg, 56%).

ETTE: M.p.= 126°C; ^{1}H NMR ($CDCl_3$): δ = 0.89 (t, ^{3}J = 6.9 Hz, 6H), 1.34 (m, 12H), 1.6 (m, 4H), 2.64 (t, ^{3}J = 7.6 Hz, 4H), 4.23 (m, 4H), 4.33 (m, 4H), 7.01 (d, ^{3}J = 3.8 Hz, 2H), 7.03 (d, ^{3}J = 3.8 Hz, 2H); ^{13}C NMR ($CDCl_3$): δ =14.05, 22.54, 25.71, 28.75, 30.32, 31.50, 64.47, 65.09, 107.92, 116.44, 122.44, 123.03, 133.72, 134.94, 137.37, 137.52; HRMS calculated for $C_{32}H_{38}O_4S_4$: 614.1653; found: 614.1642; elemental analysis calculated (%) for $C_{32}H_{38}O_4S_4$: C 62.50, H 6.23, O 10.41, S 20.86; found: C 62.29, H 6.10, O 10.51, S 20.59.

3',4',3",4"-Bis(ethylenedioxy)-5,5'''-dihexyl-2,2':5',2":5",2"'-quaterthiophene (TEET):
The distannic derivative **5c** was prepared by the same procedure described for **1b** starting from **5a** by using two equivalents of n-BuLi and a slight excess of Bu_3SnCl. The product was used without other purification for the following reaction.
The Stille coupling was done according to the procedure described for **2a** in toluene (50mL) by using 2-bromo-5-hexylthiophene (11.75mmol, 1.5 eq) **5c** (4.7mmol) and $Pd(PPh_3)_4$ (500mg). The product was purified by chromatography on silica gel (CH_2Cl_2 / EP 1/1) to give **TEET** as orange solid (1.41g, 56%).
TEET: M.p.=150°C; ^{1}H NMR ($CDCl_3$): δ = 0.88 (t, ^{3}J = 6.9 Hz, 6H), 1.34 (m, 12H), 1.67 (m, 4H), 2.79 (t, ^{3}J = 7.4 Hz, 4H), 4.38 (m, 8H), 6.68 (d, ^{3}J = 3.5 Hz, 2H), 7.03 (d, ^{3}J = 3.5 Hz, 2H); ^{13}C NMR ($CDCl_3$): δ = 14.07, 22.56, 28.77, 30.11, 31.56, 31.61, 64.93, 65.03, 106.95, 110.65, 122.28, 124.16, 132.13, 136.48, 136.91, 144.57; HRMS calculated for $C_{32}H_{38}O_4S_4$: 614.1653; found: 614.1652; elemental analysis calculated (%) for $C_{32}H_{38}O_4S_4$: C 62.50, H 6.23, O 10.41; found: C 62.76, H 6.11, O 10.45.

5-Hexyl- 3',4'-ethylenedioxy-2,2':5',2''terthiophene (8a) :
The stannic derivative **2b** was prepared by the same procedure described for **1b** starting from **2a**. The product was used without other purification for the Stille coupling reaction.
The Stille coupling was done according to the procedure described for **2a** in toluene (50mL) by using **2b** (12.76mmol), 2-bromo-5-hexyl-thiophene (2.88g, 11.6mmol) and $Pd(PPh_3)_4$ (680mg). The product was purified by chromatography on silica gel (CH_2Cl_2 / EP 1/2) to obtain **8a** as yellow oil (2.8g, 55%).
8a: ^{1}H NMR ($CDCl_3$): δ = 0.9 (t, ^{3}J = 6.8 Hz, 3H), 1.34 (m, 6H), 1.68 (m, 2H), 2.79 (t, ^{3}J = 7.5 Hz, 2H), 4.39 (m, 4H), 6.68 (d, ^{3}J = 3.5 Hz, 1H), 7.01 (d, ^{3}J = 3.5 Hz, 1H), 7.02 (m, 1H); 7.24 (m, 2H); MS (MALDI-TOF) calculated for $C_{20}H_{22}O_2S_3$: 390.08; found: 389.96.

5-bromo-5''-Hexyl-3',4'-ethylenedioxy-2,2':5',2''terthiophene (8b) :
NBS (374mg, 2.05mmol) was added by portion to a solution of **8a** (800mg, 2.05mmol) in $CHCl_3$ (50mL) at -20°C and under inert atmosphere (N_2), The mixture was stirred during 2h at the addition temperature then 1h at room temperature. The solution was concentrated and the residue was dissolved in CH_2Cl_2. After washing with water, the organic phase was dried on $MgSO_4$ and then concentrated. A flash-chromatography on silica gel was carried out with a mixture CH_2Cl_2 / EP (1/1). The product was recristallized in a $CHCl_3$ / absolute ethanol to obtain **8b** as yellow crystals (270mg, 28%). **8b**: ^{1}H NMR ($CDCl_3$): δ = 0.89 (t, ^{3}J = 6.8 Hz, 3H), 1.32 (m, 6H), 1.68 (m, 2H), 2.76 (t, ^{3}J = 7.5 Hz, 2H), 4.37 (s, 4H), 6.68 (d, ^{3}J = 3.5 Hz, 1H), 6.94 (m, 2H), 7.01 (d, ^{3}J = 3.5 Hz, 1H); MS (MALDI-TOF) calculated for $C_{20}H_{21}BrO_2S_3$: 468.01; found: 467.81.

3,4,3",4"-Bis(ethylenedioxy)-5,5'''-dihexyl-2,2':5',2":5",2"'-quaterthiophene (TETE) : The Stille coupling was done according to the procedure described for **2a** in toluene (50mL) by using **7b** (1.70mmol), **8b** (500mg, 0.65mmol) and $Pd(PPh_3)_4$ (80mg). The product was purified by chromatography on silica gel (CH_2Cl_2 / EP 2/1) to obtain **TETE** as orange solid (80mg, 10%).
M.p.=98°C; ^{1}H NMR ($CDCl_3$): δ = 0.89 (m, 6H), 1.32 (m, 12H), 1.65 (m, 4H), 2.63 (t, ^{3}J = 7.5 Hz, 2H), 2.79 (t, ^{3}J = 7.5 Hz, 2H), 4.23 (m, 2H), 4.32 (m, 2H), 4.38 (s, 4H), 6.68 (d, ^{3}J = 3.5 Hz 1H); 7.00-7.10 (m, 3H); MS (MALDI) calculated for $C_{32}H_{38}O_4S_4$: 614.17; found: 614.04; Elemental analysis calculated (%) for $C_{32}H_{38}O_4S_4$: C 62.50, H 6.23, O 10.41; found: C 62.35, H 6.10, O 10.52.

3,4,3"',4"'-Bis(ethylenedioxy)-5,5""-dihexyl-2,2':5',2":5",2"':5"',2""-quinquithiophene (ETTTE) :

The Stille coupling was done according to the procedure described for **2a** in toluene (50mL) by using **7b** (1.05mmol), dibromoterthiophene (200mg, 0.49mmol) and $Pd(PPh_3)_4$ (60mg). The product was purified by chromatography on silica gel (CH_2Cl_2 / EP 1/1) to obtain **ETTTE** as orange solid (30mg, 18%).

ETTTE : M.p.=131°C; ^1H NMR ($CDCl_3$): δ = 0.9 (t, ^3J = 6.8 Hz, 6H), 1.33 (m, 12H), 1.60 (m, 4H), 2.64 (t, ^3J = 7.4 Hz, 4H), 4.24 (m, 4H), 4.33 (m, 4H), 7.00-7.06 (m, 6H); MS (MALDI-TOF) calculated for $C_{36}H_{40}O_4S_5$: 696.15; found: 696.04; elemental analysis calculated (%) for $C_{36}H_{40}O_4S_5$: C 62.03, H 5.78, O 9.18, S 23.00; found: C 61.74, H 5.79, O 8.97, S 22.88.

3',4',3"',4"'-Bis(ethylenedioxy)-5,5""-dihexyl-2,2':5',2":5",2"':5"',2""-quinquithiophene (TETET) :

The stannic derivative **3b** was prepared by the same procedure described for **1b** starting from **3a**. The product was used without other purification for the Stille coupling reaction.

The Stille coupling was done according to the procedure described for **2a** in toluene (50mL) by using **3b** (1.83mmol), 2,5-dibromothiophene (200mg, 0.85mmol) and $Pd(PPh_3)_4$ (100mg). The product was purified by chromatography on silica gel (CH_2Cl_2 / EP 2/1) and then recristallized in a $CHCl_3$ / absolute ethanol mixture to obtain **TETET** as orange solid (355mg, 62%).

TETET: M.p.=188°C; ^1H NMR ($CDCl_3$): δ = 0.9 (t, ^3J = 6.8 Hz, 6H), 1.34 (m, 12H), 1.68 (m, 4H), 2.79 (t, ^3J = 7.5 Hz, 4H), 4.39 (m, 8H), 6.69 (d, ^3J = 3.5 Hz, 2H), 7.03 (d, ^3J = 3.5 Hz, 2H), 7.12 (s, 2H); ^{13}C NMR ($CDCl_3$): δ = 14.07, 22.56, 28.76, 30.10, 31.55 (2), 64.90, 64.97, 109.10, 109.95, 122.64, 122.79, 124.23, 131.77, 132.84, 136.92, 137.42, 144.93; HRSM calculated for $C_{36}H_{40}O_4S_5$: 696.1530; found: 696.1531; elemental analysis calculated (%) for $C_{36}H_{40}O_4S_5$: C 62.03, H 5.78, O 9.18, S 23.00; found: C 61.97, H 5.68, O 8.71, S 23.46.

5,5""-Dihexyl-3',4',3'',4'',3"',4"'-tris(ethylenedioxy)-2,2':5',2":5",2"':5"',2""-quinquithiophene (TEEET) :

The Stille coupling was done according to the procedure described for **2a** in toluene (50mL) by using **3b** (2.86mmol), 2,5-dibromo-3,4ethylenedioxythiophene (400mg, 1.33mmol) and $Pd(PPh_3)_4$ (160mg). The product was purified by chromatography on silica gel (CH_2Cl_2 / EP 1/1 Et_3N 1%) to obtain **TEEET** as red solid (210mg, 21%).

TEEET: M.p.=212°C; ^1H NMR ($CDCl_3$): δ = 0.89 (t, ^3J = 6.4 Hz), 1.32 (m, 12H), 1.68 (m, 4H), 2.79 (t, ^3J = 7.5 Hz, 4H), 4.4 (m, 12H), 6.67 (d, ^3J = 3.4 Hz, 2H), 7.03 (d, ^3J = 3.4 Hz, 2H); HRMS calculated for $C_{38}H_{42}O_6S_5$: 754.1585; found: 754.1548; elemental analysis calculated (%) for $C_{38}H_{42}O_6S_5$: C 60.45, H 5.61, O 12.71, S 21.23;found: C 60.21, H 5.70, O 12.99, S 21.13.

5,5""-Dihexyl-3,4,3",4",3"',4"'-tris(ethylenedioxy)-2,2':5',2":5",2"':5"',2""-quinquithiophene (ETETE) :

The Stille coupling was done according to the procedure described for **2a** in toluene (50mL) by using **4b** (600mg, 1.29mmol), **7b** (2.8mmol) and $Pd(PPh_3)_4$ (150mg). The product was purified by chromatography on silica gel (CH_2Cl_2 / EP 1/1) to obtain **ETETE** as red solid (490mg, 47%).

ETETE: M.p.=214°C; ^1H NMR ($CDCl_3$): δ = 0.89 (t, ^3J = 6.8 Hz, 6H), 1.32 (m, 12H), 1.61 (m, 4H), 2.63 (t, ^3J = 7.4 Hz, 4H), 4.2 (m, 4H), 4.32 (m, 4H), 4.39 (s, 4H), 7.05 (d, ^3J = 3.8 Hz, 2H), 7.09 (d, ^3J = 3.8 Hz, 2H); ^{13}C NMR ($CDCl_3$): δ = 14.09, 22.57, 25.74, 28.79, 30.36, 31.53, 64.51, 64.96, 65.11, 108.13, 109.55, 116.27, 122.05, 122.83, 132.03, 133.71, 137.28 (2), 137.56; HRMS calculated for $C_{38}H_{42}O_6S_5$: 754.1585; found: 754.1574; elemental analysis calculated (%) for $C_{38}H_{42}O_6S_5$: C 60.45, H 5.61, O 12.71, S 21.23; found: C 60.22, H 5.65, O 13.28, S 21.08.

5,5""-Dihexyl-3,4,3',4'3''',4''',3"'',4"''-tetrakis(ethylenedioxy)-2,2':5',2":5",2"':5"',2""-quinquithiophene (EETEE) :

The stannic derivative **5b** was prepared by the same procedure described for **1b** starting from **5a**. The product was used without other purification for the Stille coupling reaction.

The Stille coupling was done according to the procedure described for **2a** in toluene (50mL) by using **5b** (0.94mmol), 2,5-dibromothiophene (106mg, 0.44mmol) and $Pd(PPh_3)_4$ (25mg). The product was purified by chromatography on silica gel (CH_2Cl_2 / EP 1/1 Et_3N 1%) to obtain **EETEE** as red solid (70mg, 20%).

EETEE: M.p.=225°C; ^1H NMR ($CDCl_3$): δ = 0.88 (t, ^3J = 6.8 Hz, 6H), 1.31 (m, 12H), 1.6 (m, 4H), 2.64 (t, ^3J = 7 Hz, 4H), 4.23 (m, 4H), 4.32 (m, 4H), 4.38 (s, 8H), 7.11 (s, 2H); Solubility was too low to measure its ^{13}C NMR spectrum. HRMS calculated for $C_{40}H_{44}O_8S_5$: 812.16397; found: 812.1635.

5,5''''''-Bis(hexyl)-3,4,3''',4''',3''''''',4''''''-tris(ethylenedioxy)-2,2':5',2'':5'',2''' :5''',2'''' :5'''',2''''',5''''',2'''''''-septithiophene (TETETET) :

The Stille coupling was done according to the procedure described for **2a** in toluene (50mL) by using **4b** (450mg, 0.97mmol), **3b** (2.08mmol) and $Pd(PPh_3)_4$ (120mg). The product was purified by soxhlet extraction using diethyl ether to remove impurities and then acetone to obtain **ETETETE** as red powder (120mg, 14%). The poor solubilty of the product did not allow to do NMR spectroscopy. M.p.>300°C; MS (MALDI-TOF) calculated for $C_{46}H_{46}O_6S_7$: 918.14; found: 918.00.

Theoretical calculations

All the theoretical calculations based on density functional methods have been performed with Gaussian98 program. Becke's three-parameter gradient-corrected functional (B3lyp) with 6-31G* basis for carbon and sulfur atoms and 6-31G for hydrogen atoms was used to optimize the geometry and to compute the electronic structure at the minima found. The determination of the dihedral angle was achieved using the Molekel-4.0 program.

The following coordinates (x, y, z) for each atoms of various oligomers, obtained after geometric optimization, inserted in a pdb file (ETTE.pdb) allow to see the geometry of the molecules by using the Chem3D Ultra 7.0 software

ETTE

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ATOM      1  C   UNK     1       4.541  -0.888  -0.054  1.00  0.00
ATOM      2  C   UNK     1       5.392   0.191   0.066  1.00  0.00
ATOM      3  C   UNK     1       6.781  -0.158   0.072  1.00  0.00
ATOM      4  C   UNK     1       6.996  -1.501  -0.046  1.00  0.00
ATOM      5  S   UNK     1       5.492  -2.366  -0.167  1.00  0.00
ATOM      6  C   UNK     1       3.100  -0.915  -0.100  1.00  0.00
ATOM      7  C   UNK     1       2.271  -2.016  -0.217  1.00  0.00
ATOM      8  C   UNK     1       0.895  -1.696  -0.249  1.00  0.00
ATOM      9  C   UNK     1       0.636  -0.342  -0.152  1.00  0.00
ATOM     10  S   UNK     1       2.139   0.556  -0.012  1.00  0.00
ATOM     11  C   UNK     1      -3.100   0.915  -0.100  1.00  0.00
ATOM     12  C   UNK     1      -2.271   2.016  -0.218  1.00  0.00
ATOM     13  C   UNK     1      -0.895   1.696  -0.249  1.00  0.00
ATOM     14  C   UNK     1      -0.636   0.342  -0.152  1.00  0.00
ATOM     15  S   UNK     1      -2.139  -0.556  -0.012  1.00  0.00
ATOM     16  C   UNK     1      -4.541   0.888  -0.054  1.00  0.00
ATOM     17  C   UNK     1      -5.392  -0.191   0.066  1.00  0.00
ATOM     18  C   UNK     1      -6.781   0.158   0.072  1.00  0.00
ATOM     19  C   UNK     1      -6.996   1.501  -0.046  1.00  0.00
ATOM     20  S   UNK     1      -5.492   2.366  -0.167  1.00  0.00
ATOM     21  O   UNK     1       4.963   1.483   0.185  1.00  0.00
ATOM     22  C   UNK     1       6.002   2.438  -0.072  1.00  0.00
ATOM     23  C   UNK     1       7.282   2.041   0.651  1.00  0.00
ATOM     24  O   UNK     1       7.769   0.783   0.171  1.00  0.00
ATOM     25  O   UNK     1      -4.963  -1.483   0.185  1.00  0.00
ATOM     26  C   UNK     1      -6.002  -2.438  -0.072  1.00  0.00
ATOM     27  C   UNK     1      -7.282  -2.041   0.651  1.00  0.00
ATOM     28  O   UNK     1      -7.769  -0.783   0.171  1.00  0.00
ATOM     29  H   UNK     1       7.942  -2.021  -0.066  1.00  0.00
ATOM     30  H   UNK     1       2.648  -3.031  -0.286  1.00  0.00
ATOM     31  H   UNK     1       0.112  -2.440  -0.352  1.00  0.00
ATOM     32  H   UNK     1      -2.648   3.031  -0.287  1.00  0.00
ATOM     33  H   UNK     1      -0.112   2.440  -0.352  1.00  0.00
ATOM     34  H   UNK     1      -7.942   2.021  -0.066  1.00  0.00
ATOM     35  H   UNK     1       5.627   3.398   0.289  1.00  0.00
ATOM     36  H   UNK     1       6.183   2.502  -1.153  1.00  0.00
ATOM     37  H   UNK     1       7.099   1.981   1.733  1.00  0.00
ATOM     38  H   UNK     1       8.077   2.767   0.462  1.00  0.00
ATOM     39  H   UNK     1      -5.627  -3.398   0.289  1.00  0.00
ATOM     40  H   UNK     1      -6.184  -2.502  -1.153  1.00  0.00
ATOM     41  H   UNK     1      -7.099  -1.982   1.733  1.00  0.00
ATOM     42  H   UNK     1      -8.077  -2.767   0.462  1.00  0.00
END
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TEET

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ATOM      1  C   UNK     1       3.251  -0.160  -0.012  1.00  0.00
ATOM      2  C   UNK     1       2.819   1.149   0.007  1.00  0.00
ATOM      3  C   UNK     1       1.405   1.295   0.024  1.00  0.00
ATOM      4  C   UNK     1       0.710   0.101   0.021  1.00  0.00
ATOM      5  S   UNK     1       1.860  -1.241  -0.004  1.00  0.00
ATOM      6  C   UNK     1      -0.710  -0.101   0.021  1.00  0.00
ATOM      7  S   UNK     1      -1.860   1.241  -0.004  1.00  0.00
ATOM      8  C   UNK     1      -3.251   0.160  -0.012  1.00  0.00
ATOM      9  C   UNK     1      -2.819  -1.149   0.007  1.00  0.00
ATOM     10  C   UNK     1      -1.405  -1.295   0.023  1.00  0.00
ATOM     11  C   UNK     1       4.597  -0.678  -0.026  1.00  0.00
ATOM     12  C   UNK     1       4.999  -2.000  -0.051  1.00  0.00
ATOM     13  C   UNK     1       6.410  -2.168  -0.049  1.00  0.00
ATOM     14  C   UNK     1       7.087  -0.979  -0.026  1.00  0.00
ATOM     15  S   UNK     1       6.007   0.378  -0.003  1.00  0.00
ATOM     16  C   UNK     1      -4.597   0.678  -0.026  1.00  0.00
ATOM     17  C   UNK     1      -4.999   2.000  -0.051  1.00  0.00
ATOM     18  C   UNK     1      -6.410   2.168  -0.050  1.00  0.00
ATOM     19  C   UNK     1      -7.087   0.979  -0.026  1.00  0.00
ATOM     20  S   UNK     1      -6.007  -0.378  -0.004  1.00  0.00
ATOM     21  O   UNK     1       3.664   2.225  -0.003  1.00  0.00
ATOM     22  C   UNK     1       3.017   3.443   0.387  1.00  0.00
ATOM     23  C   UNK     1       1.677   3.586  -0.320  1.00  0.00
ATOM     24  O   UNK     1       0.795   2.520   0.054  1.00  0.00
ATOM     25  O   UNK     1      -3.664  -2.225  -0.004  1.00  0.00
ATOM     26  C   UNK     1      -3.017  -3.443   0.387  1.00  0.00
ATOM     27  C   UNK     1      -1.677  -3.586  -0.320  1.00  0.00
ATOM     28  O   UNK     1      -0.795  -2.520   0.054  1.00  0.00
ATOM     29  H   UNK     1       4.297  -2.828  -0.070  1.00  0.00
ATOM     30  H   UNK     1       6.900  -3.136  -0.067  1.00  0.00
ATOM     31  H   UNK     1       8.156  -0.815  -0.021  1.00  0.00
ATOM     32  H   UNK     1      -4.297   2.828  -0.070  1.00  0.00
ATOM     33  H   UNK     1      -6.900   3.136  -0.067  1.00  0.00
ATOM     34  H   UNK     1      -8.156   0.815  -0.022  1.00  0.00
ATOM     35  H   UNK     1       3.697   4.251   0.108  1.00  0.00
ATOM     36  H   UNK     1       2.872   3.451   1.476  1.00  0.00
ATOM     37  H   UNK     1       1.821   3.580  -1.409  1.00  0.00
ATOM     38  H   UNK     1       1.175   4.512  -0.028  1.00  0.00
ATOM     39  H   UNK     1      -3.697  -4.251   0.107  1.00  0.00
ATOM     40  H   UNK     1      -2.872  -3.451   1.475  1.00  0.00
ATOM     41  H   UNK     1      -1.821  -3.580  -1.409  1.00  0.00
ATOM     42  H   UNK     1      -1.175  -4.512  -0.028  1.00  0.00
END
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4T

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ATOM      1  C   UNK     1      -4.623  -0.101  -0.019  1.00  0.00
ATOM      2  C   UNK     1      -5.214  -1.339  -0.168  1.00  0.00
ATOM      3  C   UNK     1      -6.632  -1.311  -0.046  1.00  0.00
ATOM      4  C   UNK     1      -7.121  -0.055   0.194  1.00  0.00
ATOM      5  S   UNK     1      -5.849   1.120   0.289  1.00  0.00
ATOM      6  C   UNK     1      -3.222   0.254  -0.081  1.00  0.00
ATOM      7  C   UNK     1      -2.643   1.498  -0.231  1.00  0.00
ATOM      8  C   UNK     1      -1.228   1.471  -0.262  1.00  0.00
ATOM      9  C   UNK     1      -0.692   0.204  -0.136  1.00  0.00
ATOM     10  S   UNK     1      -1.978  -0.978   0.051  1.00  0.00
ATOM     11  C   UNK     1       3.222  -0.254  -0.081  1.00  0.00
ATOM     12  C   UNK     1       2.643  -1.498  -0.232  1.00  0.00
ATOM     13  C   UNK     1       1.228  -1.471  -0.263  1.00  0.00
ATOM     14  C   UNK     1       0.692  -0.204  -0.137  1.00  0.00
ATOM     15  S   UNK     1       1.978   0.978   0.051  1.00  0.00
ATOM     16  C   UNK     1       4.623   0.101  -0.019  1.00  0.00
ATOM     17  C   UNK     1       5.215   1.338  -0.168  1.00  0.00
ATOM     18  C   UNK     1       6.633   1.310  -0.046  1.00  0.00
ATOM     19  C   UNK     1       7.121   0.055   0.194  1.00  0.00
ATOM     20  S   UNK     1       5.849  -1.120   0.289  1.00  0.00
ATOM     21  H   UNK     1      -4.647  -2.239  -0.377  1.00  0.00
ATOM     22  H   UNK     1      -7.262  -2.189  -0.141  1.00  0.00
ATOM     23  H   UNK     1      -8.150   0.253   0.322  1.00  0.00
ATOM     24  H   UNK     1      -3.225   2.407  -0.343  1.00  0.00
ATOM     25  H   UNK     1      -0.617   2.357  -0.399  1.00  0.00
ATOM     26  H   UNK     1       3.225  -2.407  -0.344  1.00  0.00
ATOM     27  H   UNK     1       0.617  -2.357  -0.401  1.00  0.00
ATOM     28  H   UNK     1       4.647   2.239  -0.379  1.00  0.00
ATOM     29  H   UNK     1       7.262   2.189  -0.142  1.00  0.00
ATOM     30  H   UNK     1       8.150  -0.253   0.323  1.00  0.00
END
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4E

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ATOM      1  C   UNK     1      -4.605   0.651   0.012  1.00  0.00
ATOM      2  C   UNK     1      -5.390  -0.486   0.022  1.00  0.00
ATOM      3  C   UNK     1      -6.796  -0.229   0.009  1.00  0.00
ATOM      4  C   UNK     1      -7.094   1.103  -0.012  1.00  0.00
ATOM      5  S   UNK     1      -5.651   2.073  -0.014  1.00  0.00
ATOM      6  C   UNK     1      -3.169   0.743   0.009  1.00  0.00
ATOM      7  C   UNK     1      -2.389   1.882  -0.003  1.00  0.00
ATOM      8  C   UNK     1      -0.993   1.633  -0.020  1.00  0.00
ATOM      9  C   UNK     1      -0.656   0.293  -0.021  1.00  0.00
ATOM     10  S   UNK     1      -2.128  -0.682  -0.001  1.00  0.00
ATOM     11  C   UNK     1       3.169  -0.743   0.009  1.00  0.00
ATOM     12  C   UNK     1       2.389  -1.882  -0.003  1.00  0.00
ATOM     13  C   UNK     1       0.993  -1.633  -0.020  1.00  0.00
ATOM     14  C   UNK     1       0.656  -0.293  -0.020  1.00  0.00
ATOM     15  S   UNK     1       2.128   0.682  -0.001  1.00  0.00
ATOM     16  C   UNK     1       4.605  -0.651   0.012  1.00  0.00
ATOM     17  C   UNK     1       5.390   0.486   0.022  1.00  0.00
ATOM     18  C   UNK     1       6.796   0.229   0.009  1.00  0.00
ATOM     19  C   UNK     1       7.094  -1.103  -0.012  1.00  0.00
ATOM     20  S   UNK     1       5.651  -2.073  -0.014  1.00  0.00
ATOM     21  O   UNK     1      -2.907   3.151   0.012  1.00  0.00
ATOM     22  C   UNK     1      -1.951   4.143  -0.374  1.00  0.00
ATOM     23  C   UNK     1      -0.623   3.909   0.333  1.00  0.00
ATOM     24  O   UNK     1      -0.068   2.645  -0.047  1.00  0.00
ATOM     25  O   UNK     1       2.907  -3.151   0.013  1.00  0.00
ATOM     26  C   UNK     1       1.951  -4.143  -0.375  1.00  0.00
ATOM     27  C   UNK     1       0.623  -3.909   0.333  1.00  0.00
ATOM     28  O   UNK     1       0.068  -2.645  -0.047  1.00  0.00
ATOM     29  O   UNK     1       4.879   1.757   0.054  1.00  0.00
ATOM     30  C   UNK     1       5.843   2.745  -0.325  1.00  0.00
ATOM     31  C   UNK     1       7.168   2.498   0.383  1.00  0.00
ATOM     32  O   UNK     1       7.724   1.237  -0.001  1.00  0.00
ATOM     33  O   UNK     1      -4.879  -1.757   0.054  1.00  0.00
ATOM     34  C   UNK     1      -5.843  -2.745  -0.325  1.00  0.00
ATOM     35  C   UNK     1      -7.168  -2.498   0.383  1.00  0.00
ATOM     36  O   UNK     1      -7.724  -1.237  -0.001  1.00  0.00
ATOM     37  H   UNK     1      -8.073   1.560  -0.023  1.00  0.00
ATOM     38  H   UNK     1       8.073  -1.560  -0.023  1.00  0.00
ATOM     39  H   UNK     1      -2.381   5.108  -0.092  1.00  0.00
ATOM     40  H   UNK     1      -1.807   4.115  -1.463  1.00  0.00
ATOM     41  H   UNK     1      -0.766   3.938   1.422  1.00  0.00
ATOM     42  H   UNK     1       0.114   4.663   0.046  1.00  0.00
ATOM     43  H   UNK     1       2.381  -5.108  -0.093  1.00  0.00
ATOM     44  H   UNK     1       1.807  -4.115  -1.463  1.00  0.00
ATOM     45  H   UNK     1       0.766  -3.939   1.421  1.00  0.00
ATOM     46  H   UNK     1      -0.114  -4.663   0.045  1.00  0.00
ATOM     47  H   UNK     1       5.418   3.711  -0.038  1.00  0.00
ATOM     48  H   UNK     1       5.988   2.723  -1.414  1.00  0.00
ATOM     49  H   UNK     1       7.020   2.525   1.472  1.00  0.00
ATOM     50  H   UNK     1       7.907   3.255   0.104  1.00  0.00
ATOM     51  H   UNK     1      -5.418  -3.711  -0.038  1.00  0.00
ATOM     52  H   UNK     1      -5.988  -2.723  -1.414  1.00  0.00
ATOM     53  H   UNK     1      -7.020  -2.525   1.472  1.00  0.00
ATOM     54  H   UNK     1      -7.907  -3.255   0.104  1.00  0.00
END
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ETTTE

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ATOM      1  C   UNK     1      -6.587  -0.564   0.075  1.00  0.00
ATOM      2  C   UNK     1      -7.179   0.677  -0.030  1.00  0.00
ATOM      3  C   UNK     1      -8.610   0.648   0.004  1.00  0.00
ATOM      4  C   UNK     1      -9.115  -0.613   0.140  1.00  0.00
ATOM      5  S   UNK     1      -7.840  -1.793   0.228  1.00  0.00
ATOM      6  C   UNK     1      -5.188  -0.913   0.078  1.00  0.00
ATOM      7  C   UNK     1      -4.625  -2.174   0.159  1.00  0.00
ATOM      8  C   UNK     1      -3.212  -2.171   0.152  1.00  0.00
ATOM      9  C   UNK     1      -2.658  -0.907   0.063  1.00  0.00
ATOM     10  S   UNK     1      -3.925   0.308  -0.018  1.00  0.00
ATOM     11  C   UNK     1       1.268  -0.527  -0.032  1.00  0.00
ATOM     12  C   UNK     1       0.707   0.736  -0.020  1.00  0.00
ATOM     13  C   UNK     1      -0.707   0.736   0.015  1.00  0.00
ATOM     14  C   UNK     1      -1.268  -0.527   0.030  1.00  0.00
ATOM     15  S   UNK     1       0.000  -1.746   0.001  1.00  0.00
ATOM     16  C   UNK     1       2.658  -0.907  -0.064  1.00  0.00
ATOM     17  C   UNK     1       3.212  -2.170  -0.154  1.00  0.00
ATOM     18  C   UNK     1       4.625  -2.174  -0.161  1.00  0.00
ATOM     19  C   UNK     1       5.188  -0.913  -0.078  1.00  0.00
ATOM     20  S   UNK     1       3.925   0.308   0.018  1.00  0.00
ATOM     21  C   UNK     1       6.587  -0.564  -0.075  1.00  0.00
ATOM     22  S   UNK     1       7.840  -1.793  -0.226  1.00  0.00
ATOM     23  C   UNK     1       9.115  -0.613  -0.138  1.00  0.00
ATOM     24  C   UNK     1       8.610   0.648  -0.003  1.00  0.00
ATOM     25  C   UNK     1       7.179   0.677   0.031  1.00  0.00
ATOM     26  O   UNK     1       9.366   1.785   0.079  1.00  0.00
ATOM     27  C   UNK     1       8.624   2.900   0.586  1.00  0.00
ATOM     28  C   UNK     1       7.269   3.005  -0.099  1.00  0.00
ATOM     29  O   UNK     1       6.476   1.841   0.171  1.00  0.00
ATOM     30  O   UNK     1      -6.476   1.841  -0.171  1.00  0.00
ATOM     31  C   UNK     1      -7.269   3.005   0.099  1.00  0.00
ATOM     32  C   UNK     1      -8.624   2.900  -0.586  1.00  0.00
ATOM     33  O   UNK     1      -9.366   1.785  -0.078  1.00  0.00
ATOM     34  H   UNK     1     -10.153  -0.909   0.190  1.00  0.00
ATOM     35  H   UNK     1      -5.218  -3.080   0.224  1.00  0.00
ATOM     36  H   UNK     1      -2.615  -3.074   0.214  1.00  0.00
ATOM     37  H   UNK     1       1.302   1.643  -0.040  1.00  0.00
ATOM     38  H   UNK     1      -1.302   1.643   0.032  1.00  0.00
ATOM     39  H   UNK     1       2.615  -3.074  -0.217  1.00  0.00
ATOM     40  H   UNK     1       5.218  -3.080  -0.226  1.00  0.00
ATOM     41  H   UNK     1      10.153  -0.909  -0.187  1.00  0.00
ATOM     42  H   UNK     1       9.231   3.786   0.386  1.00  0.00
ATOM     43  H   UNK     1       8.489   2.794   1.672  1.00  0.00
ATOM     44  H   UNK     1       7.401   3.116  -1.183  1.00  0.00
ATOM     45  H   UNK     1       6.699   3.855   0.284  1.00  0.00
ATOM     46  H   UNK     1      -6.699   3.855  -0.285  1.00  0.00
ATOM     47  H   UNK     1      -7.400   3.116   1.183  1.00  0.00
ATOM     48  H   UNK     1      -8.490   2.794  -1.671  1.00  0.00
ATOM     49  H   UNK     1      -9.231   3.786  -0.385  1.00  0.00
END
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ETETE

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ATOM      1  C   UNK     1      -6.602  -0.844   0.035  1.00  0.00
ATOM      2  C   UNK     1      -7.228   0.385  -0.009  1.00  0.00
ATOM      3  C   UNK     1      -8.658   0.314   0.011  1.00  0.00
ATOM      4  C   UNK     1      -9.130  -0.965   0.075  1.00  0.00
ATOM      5  S   UNK     1      -7.823  -2.112   0.111  1.00  0.00
ATOM      6  C   UNK     1      -5.194  -1.157   0.031  1.00  0.00
ATOM      7  C   UNK     1      -4.605  -2.409   0.050  1.00  0.00
ATOM      8  C   UNK     1      -3.194  -2.374   0.053  1.00  0.00
ATOM      9  C   UNK     1      -2.667  -1.094   0.032  1.00  0.00
ATOM     10  S   UNK     1      -3.962   0.098   0.012  1.00  0.00
ATOM     11  C   UNK     1       1.280  -0.714  -0.018  1.00  0.00
ATOM     12  C   UNK     1       0.711   0.544  -0.010  1.00  0.00
ATOM     13  C   UNK     1      -0.711   0.544   0.010  1.00  0.00
ATOM     14  C   UNK     1      -1.280  -0.714   0.018  1.00  0.00
ATOM     15  S   UNK     1      -0.000  -1.927   0.000  1.00  0.00
ATOM     16  C   UNK     1       2.667  -1.094  -0.032  1.00  0.00
ATOM     17  C   UNK     1       3.194  -2.375  -0.053  1.00  0.00
ATOM     18  C   UNK     1       4.605  -2.409  -0.050  1.00  0.00
ATOM     19  C   UNK     1       5.194  -1.157  -0.031  1.00  0.00
ATOM     20  S   UNK     1       3.961   0.098  -0.012  1.00  0.00
ATOM     21  C   UNK     1       9.130  -0.965  -0.075  1.00  0.00
ATOM     22  C   UNK     1       8.658   0.314  -0.011  1.00  0.00
ATOM     23  C   UNK     1       7.228   0.385   0.010  1.00  0.00
ATOM     24  C   UNK     1       6.602  -0.843  -0.035  1.00  0.00
ATOM     25  S   UNK     1       7.823  -2.112  -0.111  1.00  0.00
ATOM     26  O   UNK     1      -6.556   1.575  -0.083  1.00  0.00
ATOM     27  C   UNK     1      -7.383   2.697   0.248  1.00  0.00
ATOM     28  C   UNK     1      -8.730   2.595  -0.453  1.00  0.00
ATOM     29  O   UNK     1      -9.444   1.434  -0.015  1.00  0.00
ATOM     30  O   UNK     1       1.441   1.700  -0.032  1.00  0.00
ATOM     31  C   UNK     1       0.675   2.848   0.352  1.00  0.00
ATOM     32  C   UNK     1      -0.675   2.848  -0.353  1.00  0.00
ATOM     33  O   UNK     1      -1.441   1.700   0.031  1.00  0.00
ATOM     34  O   UNK     1       9.444   1.434   0.015  1.00  0.00
ATOM     35  C   UNK     1       8.730   2.595   0.453  1.00  0.00
ATOM     36  C   UNK     1       7.383   2.697  -0.247  1.00  0.00
ATOM     37  O   UNK     1       6.556   1.575   0.084  1.00  0.00
ATOM     38  H   UNK     1     -10.159  -1.290   0.101  1.00  0.00
ATOM     39  H   UNK     1      -5.177  -3.330   0.062  1.00  0.00
ATOM     40  H   UNK     1      -2.578  -3.267   0.069  1.00  0.00
ATOM     41  H   UNK     1       2.578  -3.267  -0.068  1.00  0.00
ATOM     42  H   UNK     1       5.177  -3.330  -0.062  1.00  0.00
ATOM     43  H   UNK     1      10.159  -1.290  -0.102  1.00  0.00
ATOM     44  H   UNK     1      -6.835   3.584  -0.080  1.00  0.00
ATOM     45  H   UNK     1      -7.526   2.742   1.336  1.00  0.00
ATOM     46  H   UNK     1      -8.585   2.554  -1.541  1.00  0.00
ATOM     47  H   UNK     1      -9.363   3.452  -0.208  1.00  0.00
ATOM     48  H   UNK     1       1.268   3.719   0.065  1.00  0.00
ATOM     49  H   UNK     1       0.532   2.849   1.441  1.00  0.00
ATOM     50  H   UNK     1      -0.532   2.848  -1.442  1.00  0.00
ATOM     51  H   UNK     1      -1.268   3.719  -0.066  1.00  0.00
ATOM     52  H   UNK     1       9.363   3.452   0.209  1.00  0.00
ATOM     53  H   UNK     1       8.585   2.554   1.542  1.00  0.00
ATOM     54  H   UNK     1       7.525   2.742  -1.335  1.00  0.00
ATOM     55  H   UNK     1       6.835   3.584   0.081  1.00  0.00
END
```

TETET

```
ATOM      1  C   UNK     1       2.660  -0.450   0.005  1.00  0.00
ATOM      2  C   UNK     1       3.257   0.794   0.011  1.00  0.00
ATOM      3  C   UNK     1       4.680   0.759   0.001  1.00  0.00
ATOM      4  C   UNK     1       5.217  -0.510  -0.015  1.00  0.00
ATOM      5  S   UNK     1       3.911  -1.693  -0.016  1.00  0.00
ATOM      6  C   UNK     1       1.264  -0.797   0.006  1.00  0.00
ATOM      7  C   UNK     1       0.705  -2.065   0.005  1.00  0.00
ATOM      8  C   UNK     1      -0.705  -2.065  -0.005  1.00  0.00
ATOM      9  C   UNK     1      -1.264  -0.797  -0.006  1.00  0.00
ATOM     10  S   UNK     1      -0.000   0.428   0.000  1.00  0.00
ATOM     11  C   UNK     1      -5.217  -0.510   0.015  1.00  0.00
ATOM     12  C   UNK     1      -4.680   0.759  -0.001  1.00  0.00
ATOM     13  C   UNK     1      -3.257   0.794  -0.011  1.00  0.00
ATOM     14  C   UNK     1      -2.660  -0.450  -0.005  1.00  0.00
ATOM     15  S   UNK     1      -3.911  -1.693   0.015  1.00  0.00
ATOM     16  C   UNK     1      -6.599  -0.922   0.021  1.00  0.00
ATOM     17  C   UNK     1      -7.104  -2.209   0.033  1.00  0.00
ATOM     18  C   UNK     1      -8.524  -2.264   0.029  1.00  0.00
ATOM     19  C   UNK     1      -9.103  -1.024   0.014  1.00  0.00
ATOM     20  S   UNK     1      -7.919   0.243   0.006  1.00  0.00
ATOM     21  C   UNK     1       6.599  -0.922  -0.021  1.00  0.00
ATOM     22  S   UNK     1       7.919   0.243  -0.006  1.00  0.00
ATOM     23  C   UNK     1       9.103  -1.024  -0.015  1.00  0.00
ATOM     24  C   UNK     1       8.524  -2.264  -0.028  1.00  0.00
ATOM     25  C   UNK     1       7.104  -2.209  -0.033  1.00  0.00
ATOM     26  O   UNK     1       2.555   1.967   0.039  1.00  0.00
ATOM     27  C   UNK     1       3.352   3.100  -0.329  1.00  0.00
ATOM     28  C   UNK     1       4.696   3.061   0.385  1.00  0.00
ATOM     29  O   UNK     1       5.438   1.898  -0.005  1.00  0.00
ATOM     30  O   UNK     1      -5.437   1.898   0.005  1.00  0.00
ATOM     31  C   UNK     1      -4.696   3.061  -0.384  1.00  0.00
ATOM     32  C   UNK     1      -3.352   3.100   0.329  1.00  0.00
ATOM     33  O   UNK     1      -2.555   1.967  -0.039  1.00  0.00
ATOM     34  H   UNK     1       1.300  -2.972   0.009  1.00  0.00
ATOM     35  H   UNK     1      -1.300  -2.972  -0.009  1.00  0.00
ATOM     36  H   UNK     1      -6.470  -3.090   0.045  1.00  0.00
ATOM     37  H   UNK     1      -9.088  -3.190   0.036  1.00  0.00
ATOM     38  H   UNK     1     -10.156  -0.776   0.009  1.00  0.00
ATOM     39  H   UNK     1      10.156  -0.776  -0.009  1.00  0.00
ATOM     40  H   UNK     1       9.088  -3.190  -0.036  1.00  0.00
ATOM     41  H   UNK     1       6.470  -3.090  -0.045  1.00  0.00
ATOM     42  H   UNK     1       2.778   3.982  -0.037  1.00  0.00
ATOM     43  H   UNK     1       3.502   3.108  -1.417  1.00  0.00
ATOM     44  H   UNK     1       4.547   3.055   1.473  1.00  0.00
ATOM     45  H   UNK     1       5.313   3.920   0.110  1.00  0.00
ATOM     46  H   UNK     1      -5.313   3.920  -0.109  1.00  0.00
ATOM     47  H   UNK     1      -4.547   3.055  -1.472  1.00  0.00
ATOM     48  H   UNK     1      -3.502   3.108   1.417  1.00  0.00
ATOM     49  H   UNK     1      -2.778   3.982   0.037  1.00  0.00
END
```

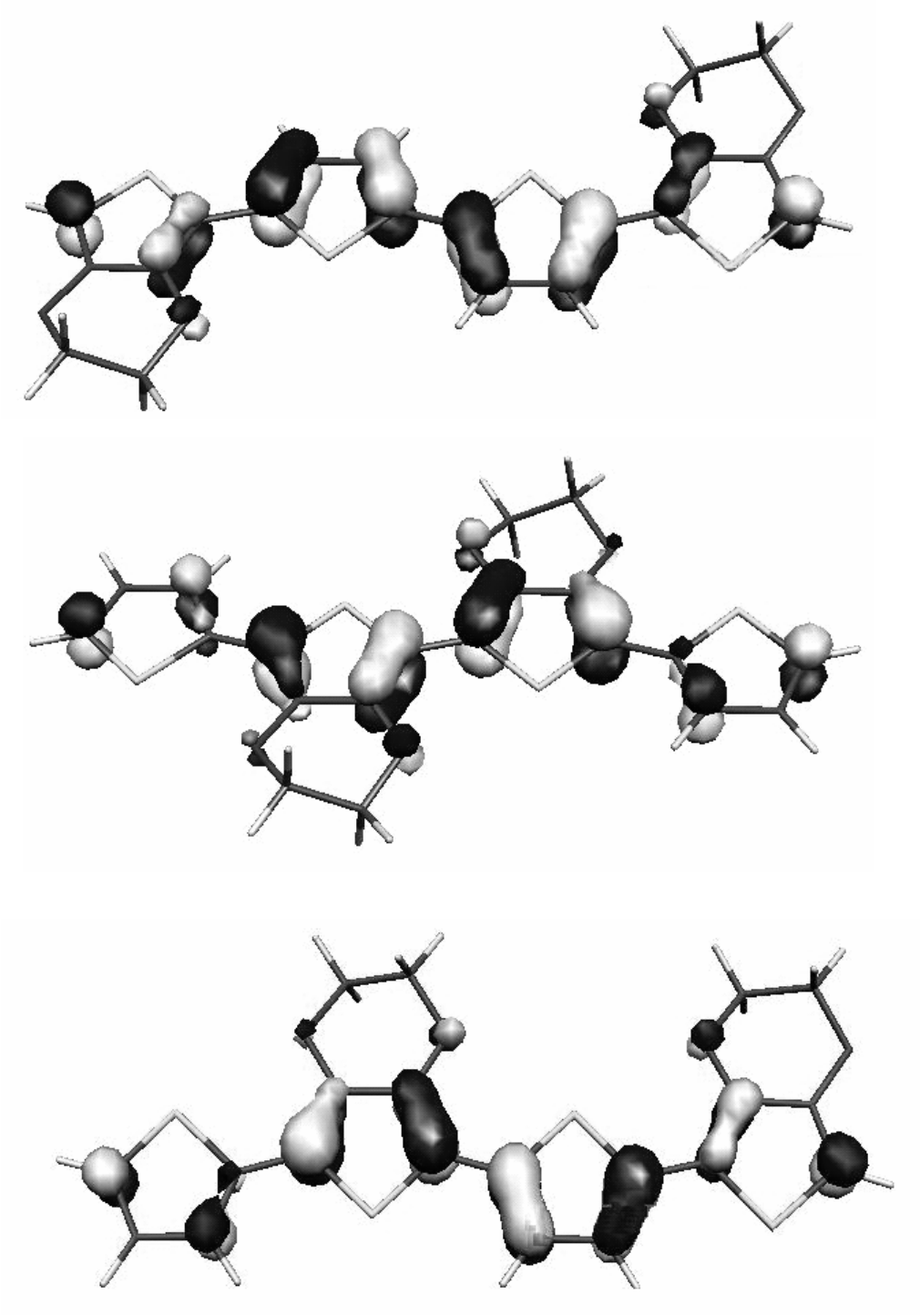
TEEET

```
ATOM      1  C   UNK     1      -6.615  -0.498   0.021  1.00  0.00
ATOM      2  C   UNK     1      -7.147  -1.775   0.038  1.00  0.00
ATOM      3  C   UNK     1      -8.569  -1.801   0.037  1.00  0.00
ATOM      4  C   UNK     1      -9.123  -0.550   0.021  1.00  0.00
ATOM      5  S   UNK     1      -7.913   0.693   0.006  1.00  0.00
ATOM      6  C   UNK     1      -5.225  -0.116   0.009  1.00  0.00
ATOM      7  C   UNK     1      -4.665   1.145  -0.011  1.00  0.00
ATOM      8  C   UNK     1      -3.245   1.150  -0.029  1.00  0.00
ATOM      9  C   UNK     1      -2.670  -0.107  -0.021  1.00  0.00
ATOM     10  S   UNK     1      -3.947  -1.327   0.005  1.00  0.00
ATOM     11  C   UNK     1       1.276  -0.449   0.019  1.00  0.00
ATOM     12  C   UNK     1       0.708  -1.710   0.012  1.00  0.00
ATOM     13  C   UNK     1      -0.708  -1.710  -0.011  1.00  0.00
ATOM     14  C   UNK     1      -1.276  -0.449  -0.018  1.00  0.00
ATOM     15  S   UNK     1       0.000   0.771   0.000  1.00  0.00
ATOM     16  C   UNK     1       2.670  -0.107   0.022  1.00  0.00
ATOM     17  C   UNK     1       3.245   1.150   0.029  1.00  0.00
ATOM     18  C   UNK     1       4.665   1.145   0.012  1.00  0.00
ATOM     19  C   UNK     1       5.225  -0.116  -0.009  1.00  0.00
ATOM     20  S   UNK     1       3.947  -1.327  -0.005  1.00  0.00
ATOM     21  C   UNK     1       9.123  -0.550  -0.023  1.00  0.00
ATOM     22  C   UNK     1       8.569  -1.801  -0.037  1.00  0.00
ATOM     23  C   UNK     1       7.147  -1.775  -0.037  1.00  0.00
ATOM     24  C   UNK     1       6.615  -0.498  -0.021  1.00  0.00
ATOM     25  S   UNK     1       7.913   0.693  -0.008  1.00  0.00
ATOM     26  O   UNK     1      -5.400   2.299  -0.003  1.00  0.00
ATOM     27  C   UNK     1      -4.637   3.447  -0.392  1.00  0.00
ATOM     28  C   UNK     1      -3.289   3.456   0.315  1.00  0.00
ATOM     29  O   UNK     1      -2.517   2.310  -0.062  1.00  0.00
ATOM     30  O   UNK     1       1.441  -2.867   0.034  1.00  0.00
ATOM     31  C   UNK     1       0.675  -4.014  -0.352  1.00  0.00
ATOM     32  C   UNK     1      -0.675  -4.014   0.352  1.00  0.00
ATOM     33  O   UNK     1      -1.441  -2.867  -0.033  1.00  0.00
ATOM     34  O   UNK     1       2.517   2.310   0.063  1.00  0.00
ATOM     35  C   UNK     1       3.289   3.456  -0.314  1.00  0.00
ATOM     36  C   UNK     1       4.637   3.447   0.393  1.00  0.00
ATOM     37  O   UNK     1       5.400   2.299   0.003  1.00  0.00
ATOM     38  H   UNK     1      -6.532  -2.668   0.051  1.00  0.00
ATOM     39  H   UNK     1      -9.152  -2.715   0.049  1.00  0.00
ATOM     40  H   UNK     1     -10.171  -0.280   0.019  1.00  0.00
ATOM     41  H   UNK     1      10.171  -0.280  -0.021  1.00  0.00
ATOM     42  H   UNK     1       9.152  -2.715  -0.048  1.00  0.00
ATOM     43  H   UNK     1       6.532  -2.668  -0.048  1.00  0.00
ATOM     44  H   UNK     1      -5.234   4.318  -0.113  1.00  0.00
ATOM     45  H   UNK     1      -4.492   3.441  -1.481  1.00  0.00
ATOM     46  H   UNK     1      -3.434   3.463   1.403  1.00  0.00
ATOM     47  H   UNK     1      -2.699   4.329   0.024  1.00  0.00
ATOM     48  H   UNK     1       1.268  -4.886  -0.065  1.00  0.00
ATOM     49  H   UNK     1       0.533  -4.014  -1.441  1.00  0.00
ATOM     50  H   UNK     1      -0.533  -4.015   1.441  1.00  0.00
ATOM     51  H   UNK     1      -1.268  -4.886   0.065  1.00  0.00
ATOM     52  H   UNK     1       2.699   4.329  -0.023  1.00  0.00
ATOM     53  H   UNK     1       3.433   3.463  -1.403  1.00  0.00
ATOM     54  H   UNK     1       4.492   3.441   1.481  1.00  0.00
ATOM     55  H   UNK     1       5.234   4.318   0.113  1.00  0.00
END
```

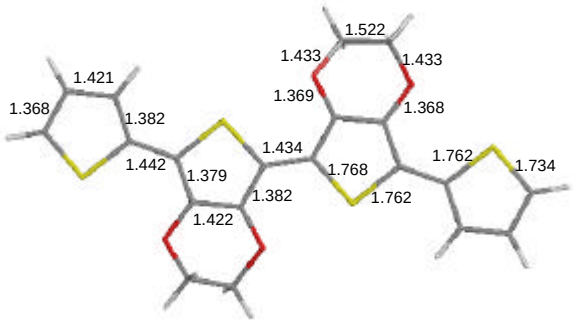
EETEE

```
ATOM      1  C   UNK     1       6.604  -0.177   0.003  1.00  0.00
ATOM      2  C   UNK     1       7.144  -1.448  -0.045  1.00  0.00
ATOM      3  C   UNK     1       8.572  -1.480  -0.013  1.00  0.00
ATOM      4  C   UNK     1       9.131  -0.237   0.060  1.00  0.00
ATOM      5  S   UNK     1       7.913   1.004   0.090  1.00  0.00
ATOM      6  C   UNK     1       5.217   0.202   0.003  1.00  0.00
ATOM      7  C   UNK     1       4.677   1.472   0.041  1.00  0.00
ATOM      8  C   UNK     1       3.256   1.506   0.050  1.00  0.00
ATOM      9  C   UNK     1       2.661   0.261   0.019  1.00  0.00
ATOM     10  S   UNK     1       3.909  -0.984  -0.026  1.00  0.00
ATOM     11  C   UNK     1      -1.265  -0.085  -0.014  1.00  0.00
ATOM     12  C   UNK     1      -0.705  -1.352  -0.009  1.00  0.00
ATOM     13  C   UNK     1       0.705  -1.352   0.009  1.00  0.00
ATOM     14  C   UNK     1       1.265  -0.085   0.014  1.00  0.00
ATOM     15  S   UNK     1      -0.000   1.139  -0.000  1.00  0.00
ATOM     16  C   UNK     1      -2.661   0.261  -0.020  1.00  0.00
ATOM     17  C   UNK     1      -3.256   1.506  -0.050  1.00  0.00
ATOM     18  C   UNK     1      -4.677   1.472  -0.041  1.00  0.00
ATOM     19  C   UNK     1      -5.217   0.202  -0.003  1.00  0.00
ATOM     20  S   UNK     1      -3.909  -0.984   0.025  1.00  0.00
ATOM     21  C   UNK     1      -9.131  -0.237  -0.060  1.00  0.00
ATOM     22  C   UNK     1      -8.572  -1.480   0.013  1.00  0.00
ATOM     23  C   UNK     1      -7.144  -1.448   0.045  1.00  0.00
ATOM     24  C   UNK     1      -6.604  -0.177  -0.003  1.00  0.00
ATOM     25  S   UNK     1      -7.913   1.004  -0.090  1.00  0.00
ATOM     26  O   UNK     1       6.387  -2.586  -0.129  1.00  0.00
ATOM     27  C   UNK     1       7.127  -3.765   0.210  1.00  0.00
ATOM     28  C   UNK     1       8.484  -3.760  -0.480  1.00  0.00
ATOM     29  O   UNK     1       9.277  -2.654  -0.037  1.00  0.00
ATOM     30  O   UNK     1      -9.277  -2.654   0.037  1.00  0.00
ATOM     31  C   UNK     1      -8.484  -3.760   0.480  1.00  0.00
ATOM     32  C   UNK     1      -7.127  -3.765  -0.210  1.00  0.00
ATOM     33  O   UNK     1      -6.387  -2.586   0.129  1.00  0.00
ATOM     34  O   UNK     1       5.437   2.611   0.059  1.00  0.00
ATOM     35  C   UNK     1       4.695   3.762   0.478  1.00  0.00
ATOM     36  C   UNK     1       3.353   3.820  -0.238  1.00  0.00
ATOM     37  O   UNK     1       2.554   2.680   0.099  1.00  0.00
ATOM     38  O   UNK     1      -2.554   2.680  -0.099  1.00  0.00
ATOM     39  C   UNK     1      -3.353   3.820   0.238  1.00  0.00
ATOM     40  C   UNK     1      -4.695   3.762  -0.478  1.00  0.00
ATOM     41  O   UNK     1      -5.437   2.611  -0.059  1.00  0.00
ATOM     42  H   UNK     1      10.182   0.013   0.093  1.00  0.00
ATOM     43  H   UNK     1      -1.300  -2.260  -0.018  1.00  0.00
ATOM     44  H   UNK     1       1.300  -2.260   0.018  1.00  0.00
ATOM     45  H   UNK     1     -10.182   0.013  -0.093  1.00  0.00
ATOM     46  H   UNK     1       6.520  -4.611  -0.122  1.00  0.00
ATOM     47  H   UNK     1       7.258  -3.818   1.299  1.00  0.00
ATOM     48  H   UNK     1       8.349  -3.710  -1.569  1.00  0.00
ATOM     49  H   UNK     1       9.051  -4.661  -0.231  1.00  0.00
ATOM     50  H   UNK     1      -9.051  -4.661   0.232  1.00  0.00
ATOM     51  H   UNK     1      -8.349  -3.710   1.570  1.00  0.00
ATOM     52  H   UNK     1      -7.258  -3.818  -1.299  1.00  0.00
ATOM     53  H   UNK     1      -6.520  -4.611   0.122  1.00  0.00
ATOM     54  H   UNK     1       5.312   4.629   0.227  1.00  0.00
ATOM     55  H   UNK     1       4.542   3.728   1.565  1.00  0.00
ATOM     56  H   UNK     1       3.507   3.855  -1.325  1.00  0.00
ATOM     57  H   UNK     1       2.779   4.696   0.073  1.00  0.00
ATOM     58  H   UNK     1      -2.779   4.696  -0.073  1.00  0.00
ATOM     59  H   UNK     1      -3.507   3.855   1.325  1.00  0.00
ATOM     60  H   UNK     1      -4.542   3.728  -1.565  1.00  0.00
ATOM     61  H   UNK     1      -5.312   4.629  -0.227  1.00  0.00
END
```

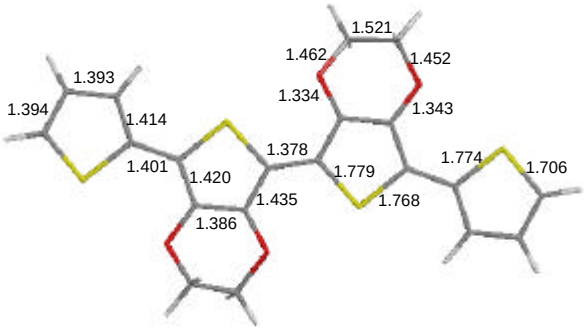
HOMO orbitals of optimized geometries for the hybrid tetramers. Top **ETTE**, middle **TEET**, bottom **ETET**.



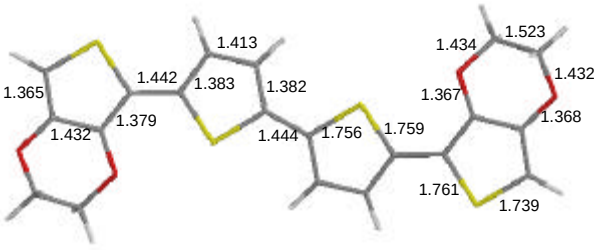
Bond lengths of TEET and ETTE for the neutral and dicationic species obtained after geometric optimization (in ?).



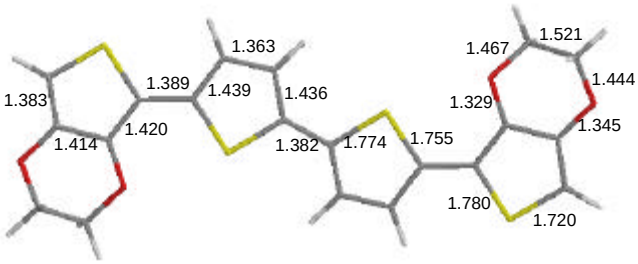
TEET



TEET- dication



ETTE



ETTE- dication