Electronic Supplementary Information

Molecular Design through the Computational Simulation on the Benzo[2,1-b;3,4-b']dithiophene-Based Highly Ordered Donor Material for Efficient Polymer Solar Cells

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Experimental section

Materials and Instruments

All reagents were purchased from Sigma Aldrich, Acros, Alfa Aesar and TCI. All chemicals were used without further purification. Toluene and tetrahydrofuran (THF) were distilled from benzophenone and sodium metal. The benzo[2,1-b:3,4-b']dithiene-4,5-diyl diacetate was synthesized by modifying the previously reported procedures.[1,2] The synthesis of 4,7-dibromo-5,6-bis(octyloxy)benzo[c][1,2,5]thiadiazole involved a multistep synthesis starting from pyrocatechol as shown in our previous paper.[3]

4,5-Di(2-ethylhexyloxy)benzo[2,1-b:3,4-b']dithiophene

Compound 1[1,2] (0.3 g, 1.14 mmol), cesium carbonate (3.5 g, 11.42 mmol), and 2-ethylhexyl bromide (3.5 mL, 11.42 mmol) were dissolved in 17.3 mL acetonitrile. The reaction mixture was stirred at 75 ^{o}C. After three days, GC/MS analysis showed the presence of intermediate. Therefore, 2-ethylhexyl bromide and cesium carbonate were added more and the mixture was refluxed to 75 ^{o}C for further 24 h. GC/MS analysis showed full conversion; the mixture was cooled to room temperature and acetonitrile was removed by rotary evaporation. The residue was partitioned between water and dichloromethane. The organic phase was washed with 2 X 100 mL 1 M HCl and then with 100 mL water, dried over Na_2SO_4 and filtered off. Evaporation of the solvent led to a brown oil. The crude product was purified by column chromatography (Flash-silica; n-hexane–DCM 1 : 1). Pure product 25 (282 0.41 g, 0.912 mmol, 80%) was obtained as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.50 (d, 2H), 7.35

(d, 2H), 4.06 (m, 4H), 1.81(m, 2H), 1.67(m, 2H), 1.55(m, 6H), 1.36(m, 8H), 0.95 (m, 13H).

2,7-Bis(trimethyltin)-4,5-di(2-ethylhexyloxy)benzo[2,1-b:3,4-b']dithiophene (M1)

4,5-di(2-ethylhexyloxy)benzo[2,1-b:3,4-b']dithiophene (0.44 g, 0.98 mmol) was dissolved in 5 mL dry THF and was degassed three times. The slightly yellow solution was cooled to -78 ^{o}C and n-BuLi (1.0 mL, 2.45 mmol, 2.5 M in hexane) was added over 20 minutes whereupon a grey suspension was formed. The suspension was stirred for 1.5 h at -78 ^{o}C and 1.5 h at room temperature. After cooling to -78 ^{o}C again, trimethylstannyl chloride 1.0M in THF (4.6 mL, 494 mg, 2.45 mmol) was added in one portion. The mixture was stirred for 1 h at -78 ^{o}C and at room temperature overnight. A light yellow solution was formed and 35 mL of n-hexane were added. The white suspension was washed with 3 X 50 mL water, dried over Na_2SO_4 and the solvent was removed in a vacuum. The crude product was dried in high vacuum to obtain 780 mg (0.68 mmol, 90%) of a colorless oil, which was used in the next step without further purification. ^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.54 (s, 2H), 4.06 (d, 4H), 1.52 (t, 4H), 1.43 (s, 2H), 1.37 (m, 10H), 0.97 (t, 8H), 0.94 (m, 8H), 0.44 (t, 24H).

10,13-dibromo-11,12-bis(octyloxy)dibenzo[a,c]phenazine

Under a nitrogen atmosphere, 4,7-dibromo-5,6-bis(octyloxy)benzo[c][1,2,5]thiadiazole[3] (1.75 g, 3.18 mmol) and zinc (2.58 g 39.4 mmol) dust were dissolved in 110 ml acetic acid. The mixture was refluxed for 3 hours at 80 °C. After cooling to room temperature, the reaction mixture was washed with a NaOH solution. The solids that resulted after the evaporation of

the organic solvent and 9,10-phenanthrenequinone (1.46 g, 7.0 mmol) were dissolved in 110 ml acetic acid. The mixture was refluxed for 1 day at 60 °C. After cooling to room temperature, an orange colored mixture was observed. After filtration, the reaction mixture was purified by column chromatography on silica gel (dichloromethane as eluent) to obtain the product as a light-yellow solid (1.3 g, 58.9 %) ^{1}H NMR (400 MHz, $CDCl_3$, δ): 9.29 (d, 2H;Ar) 8.41 (t, 2H;Ar) 7.68 (m, 4H;Ar) 4.27(t, 4H;CH_2) 1.96(t, 4H;CH_2) 1.59(m, 4H;CH_2) 1.42(m, 16H;CH_2) 0.91(t, 6H;CH_3).

11,12-bis(octyloxy)-10,13-di(thiophen-2-yl)dibenzo[a,c]phenazine

10,13-dibromo-11,12-bis(octyloxy)dibenzo[a,c]phenazine (1.0 g, 1.44 mmol) and trimethyl(thiophen-2-yl)stannane (1.35 ml, 4.3 mmol) in toluene (37 ml) was added to $PdCl_2(PPh_3)_2$ (0.101 g 0.15 mmol) under a nitrogen atmosphere. After refluxing for 48 hours at 80 °C, the mixture was cooled to room temperature and then poured into H_2O; the organic layer was extracted by $CHCl_3$ and dried over anhydrous Na_2SO_4. The crude product was purified by column chromatography on silica gel to give the product as an orange liquid (0.6 g, 59.3 %) ^{1}H NMR (400 MHz, $CDCl_3$, δ): 9.11 (d, 2H;Ar) 8.30 (t, 2H;Ar) 7.98 (t, 2H;Ar) 7.58(d, 2H;Ar) 7.53(m, 4H;Ar) 7.20(t, 2H;Ar) 3.98(t, 4H;CH_2) 1.72(m, 4H;CH_2) 1.34(m, 4H;CH_2) 1.21(m, 16H;CH_2) 0.82(t, 6H;CH_3).

10,13-bis(5-bromothiophen-2-yl)-11,12-bis(octyloxy)dibenzo[a,c]phenazine (M2)

Under a nitrogen atmosphere, 11,12-bis(octyloxy)-10,13-di(thiophen-2-yl)dibenzo[a,c]phena-

zine (0.3 g 0.427 mmol) was dissolved in 30 ml of THF, and NBS (0.174 g, 0.982 mmol) was then added in portions. The mixture was stirred for 24 h at room temperature. Then, the mixture was poured into water and extracted with chloroform. The combined organic layers were dried over Na_2SO_4, and then the solvent was removed. The crude product was purified with column chromatography to give M2 as a red liquid (0.24 g 65.4 %) ^{1}H NMR (400 MHz, $CDCl_3$, δ): 9.10 (d, 2H;Ar) 8.31 (t, 2H;Ar) 7.90 (t, 2H;Ar) 7.60(d, 4H;Ar) 7.20(m, 2H;Ar) 3.98(t, 4H;CH_2) 1.72(m, 4H;CH_2) 1.34(m, 4H;CH_2) 1.21(m, 16H;CH_2) 0.82(t, 6H;CH_3)

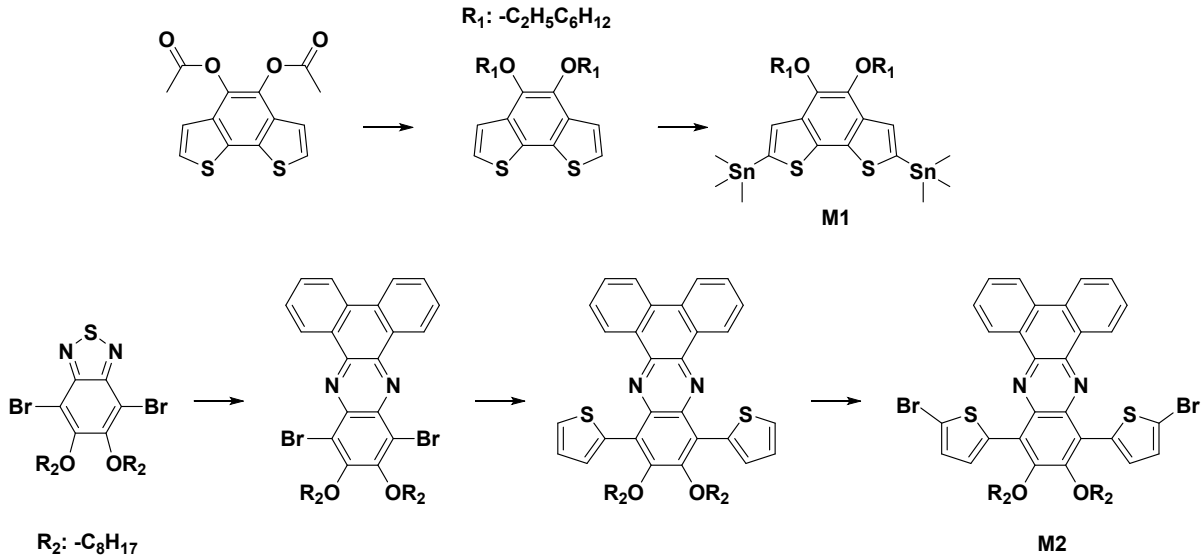

Figure S1. The Scheme routes of the monomers

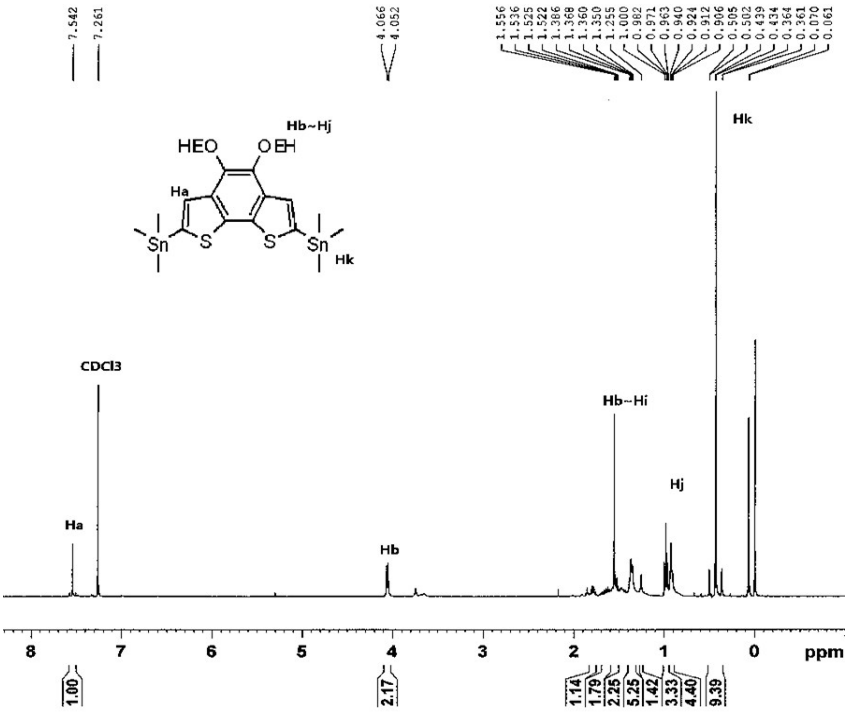

Figure S2. The ^{1}H NMR spectrum of the M1

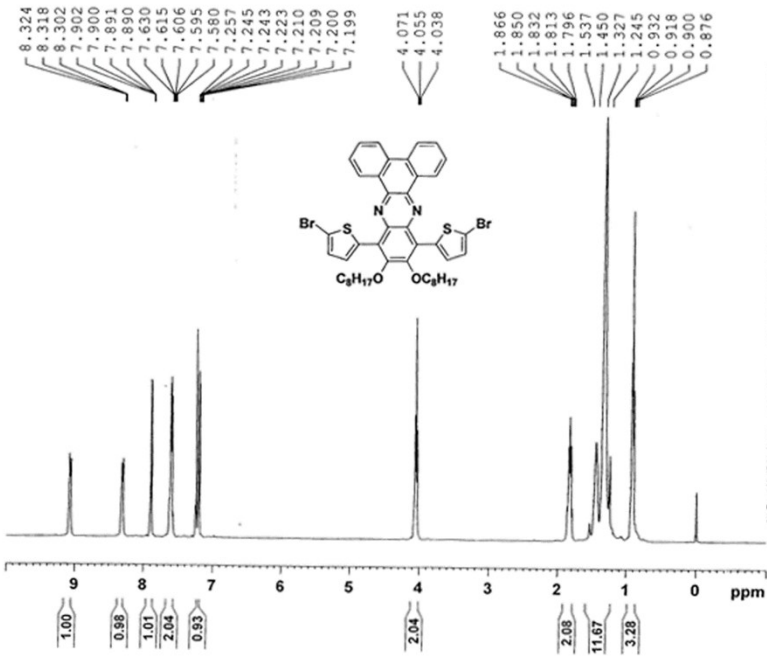

Figure S3. The ^{1}H NMR spectrum of the M2

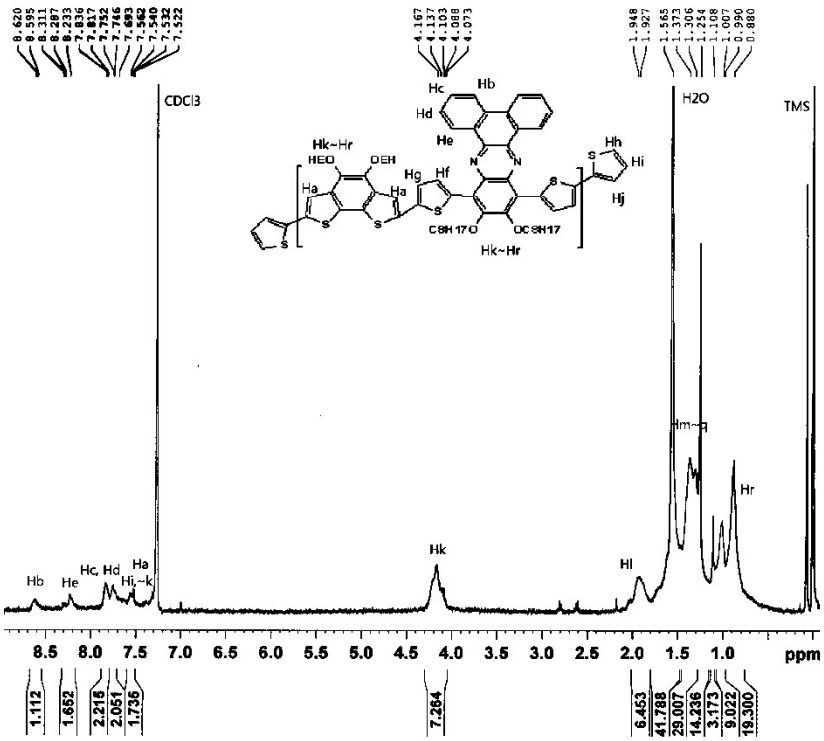

Figure S4. The ^{1}H NMR spectrum of the P(BDP-DTPz)

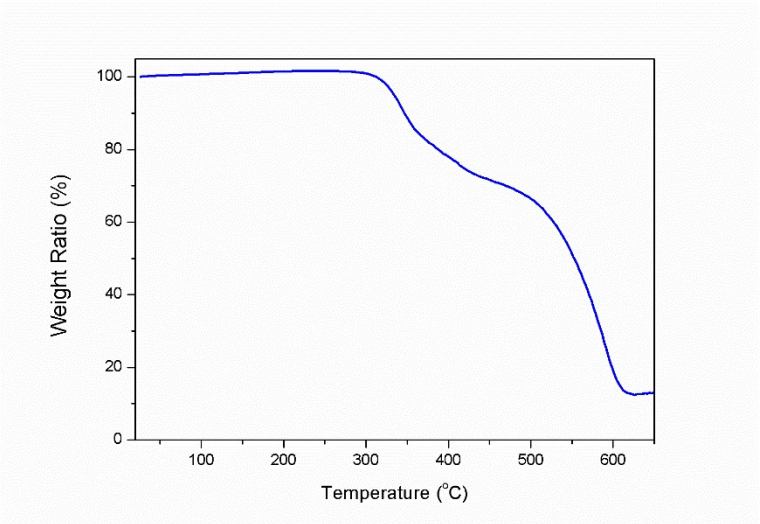

Figure S5. TGA curve of the P(BDP-DTPz)

Computational calculation data of MM & MMFF94

Figure 1. (a) BDP

----------MM2 Minimization----------

Pi System: 11 8 1 3 7 4 6 5 9 10 12 13

Warning: Some parameters are guessed (Quality = 1).

Iteration 3: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Stretch: 1.6368

Bend: 19.7789

Stretch-Bend: -0.1112

Torsion: 3.9728

Non-1,4 VDW: 1.8964

1,4 VDW: 6.5054

Dipole/Dipole: 2.9370

Total Energy: 36.6163 kcal/mol

Calculation completed

Figure 1. (b) BDP-Th (right)

----------MM2 Minimization----------

Pi System: 32 16 12 15 13 17 14 8 11 6 4 10 1 31 3 33 34

Warning: Some parameters are guessed (Quality = 1).

Iteration 2: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Stretch: 1.8261

Bend: 23.8053

Stretch-Bend: -0.2234

Torsion: 12.1154

Non-1,4 VDW: 1.7003

1,4 VDW: 6.8904

Dipole/Dipole: 3.8032

Total Energy: 49.9173 kcal/mol

Calculation completed

Figure 1. (c) BDP-Th, (right)

----------Dihedral Driver----------

Pi System: 32 16 12 15 13 17 14 8 11 6 4 10 1 31 3 33 34

Warning: Some parameters are guessed (Quality = 1).

E(-180°) = 49.92 kcal/mole

E(-175°) = 49.90 kcal/mole

E(-170°) = 49.84 kcal/mole

E(-165°) = 49.78 kcal/mole

E(-160°) = 49.72 kcal/mole

E(-155°) = 49.69 kcal/mole

E(-150°) = 49.73 kcal/mole

E(-145°) = 49.87 kcal/mole

E(-140°) = 50.14 kcal/mole

E(-135°) = 50.54 kcal/mole

E(-130°) = 51.09 kcal/mole

E(-125°) = 51.79 kcal/mole

E(-120°) = 52.63 kcal/mole

E(-115°) = 53.59 kcal/mole

E(-110°) = 54.64 kcal/mole

E(-105°) = 55.73 kcal/mole

E(-100°) = 56.83 kcal/mole

E(-95°) = 57.89 kcal/mole

E(-90°) = 58.84 kcal/mole

E(-85°) = 59.52 kcal/mole

E(-80°) = 60.02 kcal/mole

E(-75°) = 60.30 kcal/mole

E(-70°) = 60.36 kcal/mole

E(-65°) = 60.17 kcal/mole

E(-60°) = 59.74 kcal/mole

E(-55°) = 59.08 kcal/mole

E(-50°) = 58.24 kcal/mole

E(-45°) = 57.24 kcal/mole

E(-40°) = 56.13 kcal/mole

E(-35°) = 54.98 kcal/mole

E(-30°) = 53.85 kcal/mole

E(-25°) = 52.78 kcal/mole

E(-20°) = 51.84 kcal/mole

E(-15°) = 51.06 kcal/mole

E(-10°) = 50.48 kcal/mole

E(-5°) = 50.13 kcal/mole

E(0°) = 50.02 kcal/mole

E(5°) = 50.15 kcal/mole

E(10°) = 50.51 kcal/mole

E(15°) = 51.10 kcal/mole

E(20°) = 51.88 kcal/mole

E(25°) = 52.84 kcal/mole

E(30°) = 53.91 kcal/mole

E(35°) = 55.05 kcal/mole

E(40°) = 56.20 kcal/mole

E(45°) = 57.30 kcal/mole

E(50°) = 58.29 kcal/mole

E(55°) = 59.13 kcal/mole

E(60°) = 59.77 kcal/mole

E(65°) = 60.19 kcal/mole

E(70°) = 60.36 kcal/mole

E(75°) = 60.30 kcal/mole

E(80°) = 60.00 kcal/mole

E(85°) = 59.49 kcal/mole

E(90°) = 58.81 kcal/mole

E(95°) = 57.84 kcal/mole

E(100°) = 56.78 kcal/mole

E(105°) = 55.68 kcal/mole

E(110°) = 54.59 kcal/mole

E(115°) = 53.55 kcal/mole

E(120°) = 52.60 kcal/mole

E(125°) = 51.77 kcal/mole

E(130°) = 51.07 kcal/mole

E(135°) = 50.53 kcal/mole

E(140°) = 50.13 kcal/mole

E(145°) = 49.87 kcal/mole

E(150°) = 49.74 kcal/mole

E(155°) = 49.70 kcal/mole

E(160°) = 49.72 kcal/mole

E(165°) = 49.78 kcal/mole

E(170°) = 49.85 kcal/mole

E(175°) = 49.90 kcal/mole

Dihedral Driver computing finished successfully

Calculation completed

Figure 1. (d) Th-BDP-Th (left)

----------MM2 Minimization----------

Pi System: 39 29 28 27 30 2 6 1 3 5 4 7 8 10 9 11 13 12 38 37 40 41

Warning: Some parameters are guessed (Quality = 1).

Iteration 3: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Stretch: 1.8819

Bend: 27.1793

Stretch-Bend: -0.3694

Torsion: 21.0260

Non-1,4 VDW: 1.2994

1,4 VDW: 7.3100

Dipole/Dipole: 4.3404

Total Energy: 62.6675 kcal/mol

Calculation completed

Figure 1. (e) Th-BDP-Th (left)

----------Dihedral Driver----------

Pi System: 39 29 28 27 30 2 6 1 3 5 4 7 8 10 9 11 13 12 38 37 40 41

Warning: Some parameters are guessed (Quality = 1).

E(-180°) = 62.80 kcal/mole

E(-175°) = 62.75 kcal/mole

E(-170°) = 62.67 kcal/mole

E(-165°) = 62.58 kcal/mole

E(-160°) = 62.51 kcal/mole

E(-155°) = 62.49 kcal/mole

E(-150°) = 62.54 kcal/mole

E(-145°) = 62.71 kcal/mole

E(-140°) = 63.00 kcal/mole

E(-135°) = 63.45 kcal/mole

E(-130°) = 64.05 kcal/mole

E(-125°) = 64.79 kcal/mole

E(-120°) = 65.68 kcal/mole

E(-115°) = 66.67 kcal/mole

E(-110°) = 67.74 kcal/mole

E(-105°) = 68.84 kcal/mole

E(-100°) = 69.93 kcal/mole

E(-95°) = 70.96 kcal/mole

E(-90°) = 71.83 kcal/mole

E(-85°) = 72.45 kcal/mole

E(-80°) = 72.87 kcal/mole

E(-75°) = 73.08 kcal/mole

E(-70°) = 73.05 kcal/mole

E(-65°) = 72.77 kcal/mole

E(-60°) = 72.26 kcal/mole

E(-55°) = 71.53 kcal/mole

E(-50°) = 70.62 kcal/mole

E(-45°) = 69.58 kcal/mole

E(-40°) = 68.46 kcal/mole

E(-35°) = 67.31 kcal/mole

E(-30°) = 66.20 kcal/mole

E(-25°) = 65.18 kcal/mole

E(-20°) = 64.30 kcal/mole

E(-15°) = 63.61 kcal/mole

E(-10°) = 63.12 kcal/mole

E(-5°) = 62.86 kcal/mole

E(0°) = 62.84 kcal/mole

E(5°) = 63.05 kcal/mole

E(10°) = 63.50 kcal/mole

E(15°) = 64.16 kcal/mole

E(20°) = 65.02 kcal/mole

E(25°) = 66.02 kcal/mole

E(30°) = 67.13 kcal/mole

E(35°) = 68.28 kcal/mole

E(40°) = 69.42 kcal/mole

E(45°) = 70.49 kcal/mole

E(50°) = 71.44 kcal/mole

E(55°) = 72.21 kcal/mole

E(60°) = 72.78 kcal/mole

E(65°) = 73.12 kcal/mole

E(70°) = 73.21 kcal/mole

E(75°) = 73.07 kcal/mole

E(80°) = 72.70 kcal/mole

E(85°) = 72.14 kcal/mole

E(90°) = 71.36 kcal/mole

E(95°) = 70.36 kcal/mole

E(100°) = 69.30 kcal/mole

E(105°) = 68.21 kcal/mole

E(110°) = 67.14 kcal/mole

E(115°) = 66.13 kcal/mole

E(120°) = 65.23 kcal/mole

E(125°) = 64.45 kcal/mole

E(130°) = 63.82 kcal/mole

E(135°) = 63.33 kcal/mole

E(140°) = 62.99 kcal/mole

E(145°) = 62.77 kcal/mole

E(150°) = 62.67 kcal/mole

E(155°) = 62.65 kcal/mole

E(160°) = 62.69 kcal/mole

E(165°) = 62.74 kcal/mole

E(170°) = 62.79 kcal/mole

E(175°) = 62.82 kcal/mole

Dihedral Driver computing finished successfully

Calculation completed

Figure 1. (f) Pz

----------MM2 Minimization----------

Pi System: 24 19 20 21 22 18 12 6 1 2 3 5 4 9 11 10 23 15 17 16 25 26

Warning: Some parameters are guessed (Quality = 1).

Iteration 10: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Stretch: 1.6273

Bend: 6.6149

Stretch-Bend: 0.1001

Torsion: -27.0939

Non-1,4 VDW: 0.0387

1,4 VDW: 20.6972

Dipole/Dipole: 1.3977

Total Energy: 3.3819 kcal/mol

Calculation completed

Figure 1. (g) Pz-Th (right)

----------MM2 Minimization----------

Pi System: 29 24 25 22 21 20 19 17 26 16 23 9 15 10 18 11 12 5 6 1 2 4 3 28 27 30 31

Warning: Some parameters are guessed (Quality = 1).

Iteration 2: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Stretch: 1.7730

Bend: 9.2644

Stretch-Bend: -0.0814

Torsion: -11.2331

Non-1,4 VDW: -2.5826

1,4 VDW: 21.3642

Dipole/Dipole: 2.1141

Total Energy: 20.6185 kcal/mol

Calculation completed

Figure 1. (h) Pz-Th (right)

----------Dihedral Driver----------

Pi System: 29 24 25 22 21 20 19 17 26 16 23 9 15 10 18 11 12 5 6 1 2 4 3 28 27 30 31

Warning: Some parameters are guessed (Quality = 1).

E(-180°) = 43.90 kcal/mole

E(-175°) = 42.91 kcal/mole

E(-170°) = 40.53 kcal/mole

E(-165°) = 37.00 kcal/mole

E(-160°) = 32.95 kcal/mole

E(-155°) = 29.07 kcal/mole

E(-150°) = 25.83 kcal/mole

E(-145°) = 23.42 kcal/mole

E(-140°) = 21.81 kcal/mole

E(-135°) = 20.82 kcal/mole

E(-130°) = 20.32 kcal/mole

E(-125°) = 20.15 kcal/mole

E(-120°) = 20.20 kcal/mole

E(-115°) = 20.37 kcal/mole

E(-110°) = 20.59 kcal/mole

E(-105°) = 20.83 kcal/mole

E(-100°) = 21.06 kcal/mole

E(-95°) = 21.27 kcal/mole

E(-90°) = 21.45 kcal/mole

E(-85°) = 21.60 kcal/mole

E(-80°) = 21.78 kcal/mole

E(-75°) = 22.05 kcal/mole

E(-70°) = 22.46 kcal/mole

E(-65°) = 23.02 kcal/mole

E(-60°) = 23.78 kcal/mole

E(-55°) = 24.70 kcal/mole

E(-50°) = 25.77 kcal/mole

E(-45°) = 26.94 kcal/mole

E(-40°) = 28.21 kcal/mole

E(-35°) = 29.64 kcal/mole

E(-30°) = 31.34 kcal/mole

E(-25°) = 33.48 kcal/mole

E(-20°) = 36.10 kcal/mole

E(-15°) = 39.04 kcal/mole

E(-10°) = 41.77 kcal/mole

E(-5°) = 43.49 kcal/mole

E(0°) = 43.51 kcal/mole

E(5°) = 41.67 kcal/mole

E(10°) = 38.41 kcal/mole

E(15°) = 34.54 kcal/mole

E(20°) = 30.79 kcal/mole

E(25°) = 27.62 kcal/mole

E(30°) = 25.16 kcal/mole

E(35°) = 23.40 kcal/mole

E(40°) = 22.23 kcal/mole

E(45°) = 21.53 kcal/mole

E(50°) = 21.18 kcal/mole

E(55°) = 21.08 kcal/mole

E(60°) = 21.16 kcal/mole

E(65°) = 21.34 kcal/mole

E(70°) = 21.55 kcal/mole

E(75°) = 21.78 kcal/mole

E(80°) = 21.97 kcal/mole

E(85°) = 22.13 kcal/mole

E(90°) = 22.25 kcal/mole

E(95°) = 22.32 kcal/mole

E(100°) = 22.47 kcal/mole

E(105°) = 22.84 kcal/mole

E(110°) = 23.67 kcal/mole

E(115°) = 25.25 kcal/mole

E(120°) = 27.91 kcal/mole

E(125°) = 31.84 kcal/mole

E(130°) = 36.79 kcal/mole

E(135°) = 41.91 kcal/mole

E(140°) = 45.94 kcal/mole

E(145°) = 47.87 kcal/mole

E(150°) = 47.62 kcal/mole

E(155°) = 46.06 kcal/mole

E(160°) = 44.41 kcal/mole

E(165°) = 43.48 kcal/mole

E(170°) = 43.44 kcal/mole

E(175°) = 43.83 kcal/mole

Dihedral Driver computing finished successfully

Calculation completed

Figure 1. (i) Th-Pz-th (left)

----------MM2 Minimization----------

Pi System: 34 30 29 28 31 21 20 23 24 25 26 16 19 17 22 12 18 11 15 10 9 4 27 3 2 1 5 6 33 32 35 36

Warning: Some parameters are guessed (Quality = 1).

Iteration 7: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Stretch: 2.1296

Bend: 16.2045

Stretch-Bend: -0.2599

Torsion: 4.7684

Non-1,4 VDW: -4.3812

1,4 VDW: 21.5401

Dipole/Dipole: 2.1580

Total Energy: 42.1597 kcal/mol

Calculation completed

Figure 1. (j) Th-Pz-th (left)

----------Dihedral Driver----------

Pi System: 34 30 29 28 31 21 20 23 24 25 26 16 19 17 22 12 18 11 15 10 9 4 27 3 2 1 5 6 33 32 35 36

Warning: Some parameters are guessed (Quality = 1).

E(-180°) = 265.64 kcal/mole

E(-175°) = 266.15 kcal/mole

E(-170°) = 252.55 kcal/mole

E(-165°) = 226.83 kcal/mole

E(-160°) = 194.39 kcal/mole

E(-155°) = 161.44 kcal/mole

E(-150°) = 133.14 kcal/mole

E(-145°) = 109.45 kcal/mole

E(-140°) = 90.98 kcal/mole

E(-135°) = 76.88 kcal/mole

E(-130°) = 66.28 kcal/mole

E(-125°) = 58.44 kcal/mole

E(-120°) = 52.76 kcal/mole

E(-115°) = 48.77 kcal/mole

E(-110°) = 46.06 kcal/mole

E(-105°) = 44.29 kcal/mole

E(-100°) = 43.18 kcal/mole

E(-95°) = 42.52 kcal/mole

E(-90°) = 42.17 kcal/mole

E(-85°) = 42.02 kcal/mole

E(-80°) = 42.03 kcal/mole

E(-75°) = 42.20 kcal/mole

E(-70°) = 42.56 kcal/mole

E(-65°) = 43.20 kcal/mole

E(-60°) = 44.31 kcal/mole

E(-55°) = 46.19 kcal/mole

E(-50°) = 49.38 kcal/mole

E(-45°) = 54.80 kcal/mole

E(-40°) = 64.14 kcal/mole

E(-35°) = 80.54 kcal/mole

E(-30°) = 104.69 kcal/mole

E(-25°) = 154.14 kcal/mole

E(-20°) = 229.02 kcal/mole

E(-15°) = 312.02 kcal/mole

E(-10°) = 425.22 kcal/mole

E(-5°) = 566.30 kcal/mole

E(0°) = 667.34 kcal/mole

E(5°) = 646.77 kcal/mole

E(10°) = 553.52 kcal/mole

E(15°) = 469.02 kcal/mole

E(20°) = 411.24 kcal/mole

E(25°) = 352.40 kcal/mole

E(30°) = 304.81 kcal/mole

E(35°) = 265.66 kcal/mole

E(40°) = 226.23 kcal/mole

E(45°) = 183.34 kcal/mole

E(50°) = 140.48 kcal/mole

E(55°) = 104.19 kcal/mole

E(60°) = 81.70 kcal/mole

E(65°) = 64.90 kcal/mole

E(70°) = 55.02 kcal/mole

E(75°) = 49.46 kcal/mole

E(80°) = 46.44 kcal/mole

E(85°) = 44.84 kcal/mole

E(90°) = 44.06 kcal/mole

E(95°) = 43.81 kcal/mole

E(100°) = 44.01 kcal/mole

E(105°) = 44.68 kcal/mole

E(110°) = 45.96 kcal/mole

E(115°) = 48.12 kcal/mole

E(120°) = 51.54 kcal/mole

E(125°) = 56.73 kcal/mole

E(130°) = 64.34 kcal/mole

E(135°) = 73.00 kcal/mole

E(140°) = 87.43 kcal/mole

E(145°) = 105.83 kcal/mole

E(150°) = 127.99 kcal/mole

E(155°) = 153.16 kcal/mole

E(160°) = 180.05 kcal/mole

E(165°) = 207.01 kcal/mole

E(170°) = 232.17 kcal/mole

E(175°) = 252.97 kcal/mole

Dihedral Driver computing finished successfully

Calculation completed

P(BDP-DTPz) (n = 1)

----------MM2 Minimization----------

Pi System: 39 38 37 40 26 27 24 23 22 21 19 28 18 25 11 17 12 20 13 14 6 34 8 1 2 4 3 29 30 31 33 32 76 73 62 67 72 69 71 70 74 75 77 78

Optimal bond length of 1.420Å taken from the Measurements window for [C(1)-C(2)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(8)-C(1)]

Optimal bond length of 1.355Å taken from the Measurements window for [C(1)-O(9)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(2)-C(3)]

Optimal bond length of 1.355Å taken from the Measurements window for [C(2)-O(10)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(3)-C(4)]

Optimal bond length of 1.503Å taken from the Measurements window for [C(3)-C(29)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(4)-C(6)]

Optimal bond length of 1.358Å taken from the Measurements window for [C(4)-N(11)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(6)-C(8)]

Optimal bond length of 1.358Å taken from the Measurements window for [N(14)-C(6)]

Optimal bond length of 1.503Å taken from the Measurements window for [C(8)-C(34)]

Optimal bond length of 1.396Å taken from the Measurements window for [O(9)-C(16)]

Optimal bond length of 1.396Å taken from the Measurements window for [O(10)-C(15)]

Optimal bond length of 1.358Å taken from the Measurements window for [N(11)-C(12)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(12)-C(13)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(12)-C(17)]

Optimal bond length of 1.358Å taken from the Measurements window for [C(13)-N(14)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(20)-C(13)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(15)-H(41)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(15)-H(42)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(15)-H(43)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(16)-H(44)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(16)-H(45)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(16)-H(46)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(17)-C(18)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(17)-C(25)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(18)-C(19)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(28)-C(18)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(19)-C(20)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(19)-C(21)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(24)-C(20)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(21)-C(22)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(21)-H(47)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(22)-C(23)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(22)-H(48)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(23)-C(24)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(23)-H(49)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(24)-H(50)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(25)-C(26)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(25)-H(51)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(26)-C(27)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(26)-H(52)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(27)-C(28)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(27)-H(53)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(28)-H(54)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(29)-C(30)]

Optimal bond length of 1.658Å taken from the Measurements window for [S(33)-C(29)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(30)-C(31)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(30)-H(55)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(31)-C(32)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(31)-H(56)]

Optimal bond length of 1.658Å taken from the Measurements window for [C(32)-S(33)]

Optimal bond length of 1.503Å taken from the Measurements window for [C(32)-C(77)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(34)-C(37)]

Optimal bond length of 1.658Å taken from the Measurements window for [S(40)-C(34)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(37)-C(38)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(37)-H(58)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(38)-C(39)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(38)-H(60)]

Optimal bond length of 1.658Å taken from the Measurements window for [C(39)-S(40)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(39)-H(61)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(62)-H(65)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(62)-C(67)]

Optimal bond length of 1.658Å taken from the Measurements window for [S(71)-C(62)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(67)-C(69)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(67)-H(83)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(69)-C(70)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(69)-C(72)]

Optimal bond length of 1.658Å taken from the Measurements window for [C(70)-S(71)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(75)-C(70)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(72)-C(73)]

Optimal bond length of 1.355Å taken from the Measurements window for [C(72)-O(79)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(73)-C(74)]

Optimal bond length of 1.355Å taken from the Measurements window for [C(73)-O(80)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(74)-C(75)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(74)-C(76)]

Optimal bond length of 1.658Å taken from the Measurements window for [S(78)-C(75)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(76)-C(77)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(76)-H(84)]

Optimal bond length of 1.658Å taken from the Measurements window for [C(77)-S(78)]

Optimal bond length of 1.396Å taken from the Measurements window for [O(79)-C(81)]

Optimal bond length of 1.396Å taken from the Measurements window for [O(80)-C(82)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(81)-H(85)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(81)-H(86)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(81)-H(87)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(82)-H(88)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(82)-H(89)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(82)-H(90)]

Warning: Some parameters are guessed (Quality = 1).

Iteration 50: Minimization terminated normally because of an insignificant change in the varying measurements

Stretch: 0.0053

Bend: 27.1931

Stretch-Bend: -0.0001

Torsion: 29.9719

Non-1,4 VDW: -11.1229

1,4 VDW: 30.4885

Dipole/Dipole: 6.3631

Total Energy: 82.8989 kcal/mol

Calculation completed

P(BDP-DTPz) (n=1), torsion between BDP and Th (right) of Pz

----------Dihedral Driver----------

Pi System: 39 38 37 40 26 27 24 23 22 21 19 28 18 25 11 17 12 20 13 14 6 34 8 1 2 4 3 29 30 31 33 32 76 73 62 67 72 69 71 70 74 75 77 78

Warning: Some parameters are guessed (Quality = 1).

E(-180°) = 109.98 kcal/mole

E(-175°) = 109.60 kcal/mole

E(-170°) = 109.20 kcal/mole

E(-165°) = 108.84 kcal/mole

E(-160°) = 108.56 kcal/mole

E(-155°) = 108.40 kcal/mole

E(-150°) = 108.40 kcal/mole

E(-145°) = 108.58 kcal/mole

E(-140°) = 108.92 kcal/mole

E(-135°) = 109.43 kcal/mole

E(-130°) = 110.10 kcal/mole

E(-125°) = 110.88 kcal/mole

E(-120°) = 111.76 kcal/mole

E(-115°) = 112.68 kcal/mole

E(-110°) = 113.60 kcal/mole

E(-105°) = 114.47 kcal/mole

E(-100°) = 115.26 kcal/mole

E(-95°) = 115.93 kcal/mole

E(-90°) = 116.43 kcal/mole

E(-85°) = 116.71 kcal/mole

E(-80°) = 116.76 kcal/mole

E(-75°) = 116.51 kcal/mole

E(-70°) = 116.15 kcal/mole

E(-65°) = 115.51 kcal/mole

E(-60°) = 114.64 kcal/mole

E(-55°) = 113.73 kcal/mole

E(-50°) = 112.68 kcal/mole

E(-45°) = 111.61 kcal/mole

E(-40°) = 110.58 kcal/mole

E(-35°) = 109.65 kcal/mole

E(-30°) = 108.88 kcal/mole

E(-25°) = 108.32 kcal/mole

E(-20°) = 107.98 kcal/mole

E(-15°) = 107.86 kcal/mole

E(-10°) = 107.94 kcal/mole

E(-5°) = 108.20 kcal/mole

E(0°) = 108.60 kcal/mole

E(5°) = 109.13 kcal/mole

E(10°) = 109.76 kcal/mole

E(15°) = 110.48 kcal/mole

E(20°) = 111.28 kcal/mole

E(25°) = 112.11 kcal/mole

E(30°) = 112.93 kcal/mole

E(35°) = 113.69 kcal/mole

E(40°) = 114.34 kcal/mole

E(45°) = 114.81 kcal/mole

E(50°) = 115.08 kcal/mole

E(55°) = 115.10 kcal/mole

E(60°) = 114.89 kcal/mole

E(65°) = 114.38 kcal/mole

E(70°) = 113.78 kcal/mole

E(75°) = 112.96 kcal/mole

E(80°) = 112.04 kcal/mole

E(85°) = 111.06 kcal/mole

E(90°) = 110.06 kcal/mole

E(95°) = 109.10 kcal/mole

E(100°) = 108.25 kcal/mole

E(105°) = 107.54 kcal/mole

E(110°) = 107.00 kcal/mole

E(115°) = 106.66 kcal/mole

E(120°) = 106.47 kcal/mole

E(125°) = 106.61 kcal/mole

E(130°) = 106.89 kcal/mole

E(135°) = 107.35 kcal/mole

E(140°) = 107.92 kcal/mole

E(145°) = 108.56 kcal/mole

E(150°) = 109.18 kcal/mole

E(155°) = 109.72 kcal/mole

E(160°) = 110.13 kcal/mole

E(165°) = 110.36 kcal/mole

E(170°) = 110.39 kcal/mole

E(175°) = 110.25 kcal/mole

Dihedral Driver computing finished successfully

Calculation completed

Total energy of P(BDP-DTPz) (n = 1): 82.8989 kcal/mol (MM) < 106.47 kcal/mole (dihedral driver) → Error! → MMFF94 & Dihedral driver

Figure 1. (k) P(BDP-DTPz) (n = 1)

----------MMFF94 Minimization----------

Iteration 2: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Final Energy: 274.938 kcal/mol

Calculation completed

Figure 1. (l) P(BDP-DTPz) (n=1), torsion between BDP and Th (right) of Pz

----------Dihedral Driver----------

Pi System: 39 38 36 40 26 27 24 23 22 21 19 28 18 25 11 17 12 20 13 14 5 34 7 1 2 4 3 29 30 31 33 32 76 73 62 66 72 68 71 70 74 75 77 78

Warning: Some parameters are guessed (Quality = 1).

E(-180°) = 150.17 kcal/mole

E(-175°) = 150.21 kcal/mole

E(-170°) = 150.22 kcal/mole

E(-165°) = 150.23 kcal/mole

E(-160°) = 150.25 kcal/mole

E(-155°) = 150.32 kcal/mole

E(-150°) = 150.47 kcal/mole

E(-145°) = 150.73 kcal/mole

E(-140°) = 151.12 kcal/mole

E(-135°) = 151.65 kcal/mole

E(-130°) = 152.35 kcal/mole

E(-125°) = 153.20 kcal/mole

E(-120°) = 154.19 kcal/mole

E(-115°) = 155.30 kcal/mole

E(-110°) = 156.50 kcal/mole

E(-105°) = 157.75 kcal/mole

E(-100°) = 158.99 kcal/mole

E(-95°) = 160.19 kcal/mole

E(-90°) = 161.28 kcal/mole

E(-85°) = 161.93 kcal/mole

E(-80°) = 162.37 kcal/mole

E(-75°) = 162.59 kcal/mole

E(-70°) = 162.58 kcal/mole

E(-65°) = 162.32 kcal/mole

E(-60°) = 161.83 kcal/mole

E(-55°) = 161.11 kcal/mole

E(-50°) = 160.21 kcal/mole

E(-45°) = 159.16 kcal/mole

E(-40°) = 158.01 kcal/mole

E(-35°) = 156.81 kcal/mole

E(-30°) = 155.63 kcal/mole

E(-25°) = 154.52 kcal/mole

E(-20°) = 153.53 kcal/mole

E(-15°) = 152.71 kcal/mole

E(-10°) = 152.10 kcal/mole

E(-5°) = 151.71 kcal/mole

E(0°) = 151.56 kcal/mole

E(5°) = 151.67 kcal/mole

E(10°) = 152.02 kcal/mole

E(15°) = 152.59 kcal/mole

E(20°) = 153.38 kcal/mole

E(25°) = 154.33 kcal/mole

E(30°) = 155.41 kcal/mole

E(35°) = 156.56 kcal/mole

E(40°) = 157.73 kcal/mole

E(45°) = 158.85 kcal/mole

E(50°) = 159.86 kcal/mole

E(55°) = 160.73 kcal/mole

E(60°) = 161.39 kcal/mole

E(65°) = 161.83 kcal/mole

E(70°) = 162.02 kcal/mole

E(75°) = 161.96 kcal/mole

E(80°) = 161.68 kcal/mole

E(85°) = 161.18 kcal/mole

E(90°) = 160.51 kcal/mole

E(95°) = 159.39 kcal/mole

E(100°) = 158.15 kcal/mole

E(105°) = 156.90 kcal/mole

E(110°) = 155.66 kcal/mole

E(115°) = 154.48 kcal/mole

E(120°) = 153.40 kcal/mole

E(125°) = 152.44 kcal/mole

E(130°) = 151.63 kcal/mole

E(135°) = 150.98 kcal/mole

E(140°) = 150.49 kcal/mole

E(145°) = 150.15 kcal/mole

E(150°) = 149.96 kcal/mole

E(155°) = 149.88 kcal/mole

E(160°) = 149.88 kcal/mole

E(165°) = 149.94 kcal/mole

E(170°) = 150.03 kcal/mole

E(175°) = 150.11 kcal/mole

Dihedral Driver computing finished successfully

Calculation completed

P(BDP-DTPz) (n = 2)

----------MM2 Minimization----------

Pi System: 39 38 37 40 26 27 24 23 22 21 19 28 18 25 11 17
12 20 13 14 6 35 8 1 2 4 3 29 30 31 33 32 85 83 82
78 75 74 68 79 70 72 66 62 134 133 132 135 123 124 121 120 119 118 116
125 115 122 108 114 109 117 110 111 104 131 105 100 101 103 102 126 127 128 130 129
164 161 154 156 160 157 159 158 162 163 165 166

Optimal bond length of 1.420Å taken from the Measurements window for [C(1)-C(2)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(8)-C(1)]

Optimal bond length of 1.355Å taken from the Measurements window for [C(1)-O(9)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(2)-C(3)]

Optimal bond length of 1.355Å taken from the Measurements window for [C(2)-O(10)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(3)-C(4)]

Optimal bond length of 1.503Å taken from the Measurements window for [C(3)-C(29)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(4)-C(6)]

Optimal bond length of 1.358Å taken from the Measurements window for [C(4)-N(11)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(6)-C(8)]

Optimal bond length of 1.358Å taken from the Measurements window for [N(14)-C(6)]

Optimal bond length of 1.503Å taken from the Measurements window for [C(8)-C(35)]

Optimal bond length of 1.396Å taken from the Measurements window for [O(9)-C(16)]

Optimal bond length of 1.396Å taken from the Measurements window for [O(10)-C(15)]

Optimal bond length of 1.358Å taken from the Measurements window for [N(11)-C(12)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(12)-C(13)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(12)-C(17)]

Optimal bond length of 1.358Å taken from the Measurements window for [C(13)-N(14)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(20)-C(13)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(15)-H(41)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(15)-H(42)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(15)-H(43)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(16)-H(44)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(16)-H(45)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(16)-H(46)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(17)-C(18)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(17)-C(25)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(18)-C(19)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(28)-C(18)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(19)-C(20)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(19)-C(21)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(24)-C(20)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(21)-C(22)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(21)-H(47)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(22)-C(23)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(22)-H(48)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(23)-C(24)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(23)-H(49)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(24)-H(50)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(25)-C(26)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(25)-H(51)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(26)-C(27)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(26)-H(52)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(27)-C(28)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(27)-H(53)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(28)-H(54)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(29)-C(30)]

Optimal bond length of 1.658Å taken from the Measurements window for [S(33)-C(29)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(30)-C(31)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(30)-H(55)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(31)-C(32)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(31)-H(56)]

Optimal bond length of 1.658Å taken from the Measurements window for [C(32)-S(33)]

Optimal bond length of 1.503Å taken from the Measurements window for [C(32)-C(83)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(35)-C(37)]

Optimal bond length of 1.658Å taken from the Measurements window for [S(40)-C(35)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(37)-C(38)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(37)-H(58)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(38)-C(39)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(38)-H(60)]

Optimal bond length of 1.658Å taken from the Measurements window for [C(39)-S(40)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(39)-H(61)]

Optimal bond length of 1.658Å taken from the Measurements window for [S(72)-C(62)]

Optimal bond length of 1.503Å taken from the Measurements window for [C(62)-C(134)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(62)-C(66)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(66)-H(92)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(66)-C(68)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(68)-C(70)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(68)-C(74)]

Optimal bond length of 1.658Å taken from the Measurements window for [C(70)-S(72)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(79)-C(70)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(74)-C(75)]

Optimal bond length of 1.355Å taken from the Measurements window for [C(74)-O(88)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(75)-C(78)]

Optimal bond length of 1.355Å taken from the Measurements window for [C(75)-O(89)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(78)-C(79)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(78)-C(82)]

Optimal bond length of 1.658Å taken from the Measurements window for [S(85)-C(79)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(82)-C(83)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(82)-H(93)]

Optimal bond length of 1.658Å taken from the Measurements window for [C(83)-S(85)]

Optimal bond length of 1.396Å taken from the Measurements window for [O(88)-C(90)]

Optimal bond length of 1.396Å taken from the Measurements window for [O(89)-C(91)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(90)-H(94)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(90)-H(95)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(90)-H(96)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(91)-H(97)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(91)-H(98)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(91)-H(99)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(100)-C(101)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(105)-C(100)]

Optimal bond length of 1.355Å taken from the Measurements window for [C(100)-O(106)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(101)-C(102)]

Optimal bond length of 1.355Å taken from the Measurements window for [C(101)-O(107)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(102)-C(103)]

Optimal bond length of 1.503Å taken from the Measurements window for [C(102)-C(126)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(103)-C(104)]

Optimal bond length of 1.358Å taken from the Measurements window for [C(103)-N(108)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(104)-C(105)]

Optimal bond length of 1.358Å taken from the Measurements window for [N(111)-C(104)]

Optimal bond length of 1.503Å taken from the Measurements window for [C(105)-C(131)]

Optimal bond length of 1.396Å taken from the Measurements window for [O(106)-C(113)]

Optimal bond length of 1.396Å taken from the Measurements window for [O(107)-C(112)]

Optimal bond length of 1.358Å taken from the Measurements window for [N(108)-C(109)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(109)-C(110)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(109)-C(114)]

Optimal bond length of 1.358Å taken from the Measurements window for [C(110)-N(111)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(117)-C(110)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(112)-H(136)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(112)-H(137)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(112)-H(138)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(113)-H(139)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(113)-H(140)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(113)-H(141)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(114)-C(115)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(114)-C(122)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(115)-C(116)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(125)-C(115)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(116)-C(117)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(116)-C(118)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(121)-C(117)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(118)-C(119)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(118)-H(142)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(119)-C(120)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(119)-H(143)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(120)-C(121)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(120)-H(144)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(121)-H(145)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(122)-C(123)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(122)-H(146)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(123)-C(124)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(123)-H(147)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(124)-C(125)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(124)-H(148)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(125)-H(149)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(126)-C(127)]

Optimal bond length of 1.658Å taken from the Measurements window for [S(130)-C(126)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(127)-C(128)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(127)-H(150)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(128)-C(129)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(128)-H(151)]

Optimal bond length of 1.658Å taken from the Measurements window for [C(129)-S(130)]

Optimal bond length of 1.503Å taken from the Measurements window for [C(129)-C(165)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(131)-C(132)]

Optimal bond length of 1.658Å taken from the Measurements window for [S(135)-C(131)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(132)-C(133)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(132)-H(152)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(133)-C(134)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(133)-H(153)]

Optimal bond length of 1.658Å taken from the Measurements window for [C(134)-S(135)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(154)-H(155)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(154)-C(156)]

Optimal bond length of 1.658Å taken from the Measurements window for [S(159)-C(154)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(156)-C(157)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(156)-H(171)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(157)-C(158)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(157)-C(160)]

Optimal bond length of 1.658Å taken from the Measurements window for [C(158)-S(159)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(163)-C(158)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(160)-C(161)]

Optimal bond length of 1.355Å taken from the Measurements window for [C(160)-O(167)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(161)-C(162)]

Optimal bond length of 1.355Å taken from the Measurements window for [C(161)-O(168)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(162)-C(163)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(162)-C(164)]

Optimal bond length of 1.658Å taken from the Measurements window for [S(166)-C(163)]

Optimal bond length of 1.420Å taken from the Measurements window for [C(164)-C(165)]

Optimal bond length of 1.100Å taken from the Measurements window for [C(164)-H(172)]

Optimal bond length of 1.658Å taken from the Measurements window for [C(165)-S(166)]

Optimal bond length of 1.396Å taken from the Measurements window for [O(167)-C(169)]

Optimal bond length of 1.396Å taken from the Measurements window for [O(168)-C(170)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(169)-H(173)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(169)-H(174)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(169)-H(175)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(170)-H(176)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(170)-H(177)]

Optimal bond length of 1.111Å taken from the Measurements window for [C(170)-H(178)]

Warning: Some parameters are guessed (Quality = 1).

Iteration 84: Minimization terminated in error because of repeated or severe errors from the line search

Stretch: 0.4388

Bend: 112.2843

Stretch-Bend: 0.0004

Torsion: 137.1867

Non-1,4 VDW: 3.2974

1,4 VDW: 83.4308

Total Energy: 336.6385 kcal/mol

Note: Due to high VDW interactions, some terms were not computed.

Calculation completed

P(BDP-DTPz) (n = 2), torsion between BDP of P(BDP-DTPz) and Th (left) of Pz

----------Dihedral Driver----------

Pi System: 39 38 37 40 26 27 24 23 22 21 19 28 18 25 11 17

12 20 13 14 6 35 8 1 2 4 3 29 30 31 33 32 85 83 82

78 75 74 68 79 70 72 66 62 134 133 132 135 123 124 121 120 119 118 116

125 115 122 108 114 109 117 110 111 104 131 105 100 101 103 102 126 127 128 130 129

164 161 154 156 160 157 159 158 162 163 165 166

Warning: Some parameters are guessed (Quality = 1).

E(-180°) = 435.01 kcal/mole

E(-175°) = 411.09 kcal/mole

E(-170°) = 392.79 kcal/mole

E(-165°) = 396.42 kcal/mole

E(-160°) = 386.77 kcal/mole

E(-155°) = 380.23 kcal/mole

E(-150°) = 376.24 kcal/mole

E(-145°) = 374.98 kcal/mole

E(-140°) = 379.10 kcal/mole

E(-135°) = 398.86 kcal/mole

E(-130°) = 445.68 kcal/mole

E(-125°) = 608.04 kcal/mole

E(-120°) = 886.70 kcal/mole

E(-115°) = 1229.44 kcal/mole

E(-110°) = 1619.64 kcal/mole

E(-105°) = 2139.96 kcal/mole

E(-100°) = 3069.52 kcal/mole

E(-95°) = 4342.26 kcal/mole

E(-90°) = 4056.22 kcal/mole

E(-85°) = 4469.92 kcal/mole

E(-80°) = 3864.56 kcal/mole

E(-75°) = 3031.67 kcal/mole

E(-70°) = 2171.84 kcal/mole

E(-65°) = 1440.11 kcal/mole

E(-60°) = 1059.20 kcal/mole

E(-55°) = 881.35 kcal/mole

E(-50°) = 799.96 kcal/mole

E(-45°) = 787.26 kcal/mole

E(-40°) = 818.86 kcal/mole

E(-35°) = 880.86 kcal/mole

E(-30°) = 974.25 kcal/mole

E(-25°) = 1096.26 kcal/mole

E(-20°) = 1253.24 kcal/mole

E(-15°) = 1459.53 kcal/mole

E(-10°) = 1759.10 kcal/mole

E(-5°) = 2151.94 kcal/mole

E(0°) = 2232.68 kcal/mole

E(5°) = 1780.94 kcal/mole

E(10°) = 1377.35 kcal/mole

E(15°) = 1148.73 kcal/mole

E(20°) = 1012.15 kcal/mole

E(25°) = 910.06 kcal/mole

E(30°) = 810.32 kcal/mole

E(35°) = 732.42 kcal/mole

E(40°) = 675.78 kcal/mole

E(45°) = 629.97 kcal/mole

E(50°) = 587.28 kcal/mole

E(55°) = 550.99 kcal/mole

E(60°) = 521.90 kcal/mole

E(65°) = 499.86 kcal/mole

E(70°) = 484.65 kcal/mole

E(75°) = 476.09 kcal/mole

E(80°) = 491.39 kcal/mole

E(85°) = 477.27 kcal/mole

E(90°) = 485.63 kcal/mole

E(95°) = 498.29 kcal/mole

E(100°) = 514.83 kcal/mole

E(105°) = 535.43 kcal/mole

E(110°) = 560.03 kcal/mole

E(115°) = 587.99 kcal/mole

E(120°) = 617.58 kcal/mole

E(125°) = 645.79 kcal/mole

E(130°) = 668.76 kcal/mole

E(135°) = 682.81 kcal/mole

E(140°) = 685.37 kcal/mole

E(145°) = 675.42 kcal/mole

E(150°) = 653.41 kcal/mole

E(155°) = 621.28 kcal/mole

E(160°) = 582.36 kcal/mole

E(165°) = 540.87 kcal/mole

E(170°) = 500.78 kcal/mole

E(175°) = 465.00 kcal/mole

Dihedral Driver computing finished successfully

Calculation completed

Total energy of P(BDP-DTPz) (n = 2): 82.8989 kcal/mol (MM) < 106.47 kcal/mole (dihedral driver) → Error! → MMFF94 & Dihedral driver

Figure 1. (m) P(BDP-DTPz) (n = 2)

----------MMFF94 Minimization----------

Iteration 3: Minimization terminated normally because the gradient norm is less than the minimum gradient norm

Final Energy: 551.532 kcal/mol

Calculation completed

Figure 1. (n) P(BDP-DTPz) (n = 2), torsion between BDP of P(BDP-DTPz) and Th (left) of Pz

----------Dihedral Driver----------

Pi System: 39 38 36 40 26 27 24 23 22 21 19 28 18 25 11 17
12 20 13 14 5 35 7 1 2 4 3 29 30 31 33 32 85 83 81
78 75 74 67 79 70 71 65 62 134 133 132 135 123 124 121 120 119 118 116
125 115 122 108 114 109 117 110 111 104 131 105 100 101 103 102 126 127 128 130 129
164 161 154 156 160 157 159 158 162 163 165 166

Warning: Some parameters are guessed (Quality = 1).

E(-180°) = 303.92 kcal/mole

E(-175°) = 303.80 kcal/mole

E(-170°) = 303.66 kcal/mole

E(-165°) = 303.53 kcal/mole

E(-160°) = 303.42 kcal/mole

E(-155°) = 303.39 kcal/mole

E(-150°) = 303.46 kcal/mole

E(-145°) = 303.63 kcal/mole

E(-140°) = 304.00 kcal/mole

E(-135°) = 304.50 kcal/mole

E(-130°) = 305.29 kcal/mole

E(-125°) = 306.35 kcal/mole

E(-120°) = 307.81 kcal/mole

E(-115°) = 309.65 kcal/mole

E(-110°) = 311.58 kcal/mole

E(-105°) = 313.10 kcal/mole

E(-100°) = 313.98 kcal/mole

E(-95°) = 314.55 kcal/mole

E(-90°) = 314.98 kcal/mole

E(-85°) = 315.36 kcal/mole

E(-80°) = 315.73 kcal/mole

E(-75°) = 315.94 kcal/mole

E(-70°) = 315.92 kcal/mole

E(-65°) = 315.63 kcal/mole

E(-60°) = 315.08 kcal/mole

E(-55°) = 314.30 kcal/mole

E(-50°) = 313.34 kcal/mole

E(-45°) = 312.23 kcal/mole

E(-40°) = 311.05 kcal/mole

E(-35°) = 309.85 kcal/mole

E(-30°) = 308.69 kcal/mole

E(-25°) = 307.63 kcal/mole

E(-20°) = 306.72 kcal/mole

E(-15°) = 306.00 kcal/mole

E(-10°) = 305.51 kcal/mole

E(-5°) = 305.25 kcal/mole

E(0°) = 305.25 kcal/mole

E(5°) = 305.49 kcal/mole

E(10°) = 305.97 kcal/mole

E(15°) = 306.67 kcal/mole

E(20°) = 307.56 kcal/mole

E(25°) = 308.60 kcal/mole

E(30°) = 309.74 kcal/mole

E(35°) = 310.93 kcal/mole

E(40°) = 312.11 kcal/mole

E(45°) = 313.21 kcal/mole

E(50°) = 314.19 kcal/mole

E(55°) = 315.00 kcal/mole

E(60°) = 315.61 kcal/mole

E(65°) = 315.99 kcal/mole

E(70°) = 316.13 kcal/mole

E(75°) = 316.04 kcal/mole

E(80°) = 315.74 kcal/mole

E(85°) = 315.24 kcal/mole

E(90°) = 314.44 kcal/mole

E(95°) = 313.36 kcal/mole

E(100°) = 312.20 kcal/mole

E(105°) = 311.00 kcal/mole

E(110°) = 309.83 kcal/mole

E(115°) = 308.71 kcal/mole

E(120°) = 307.69 kcal/mole

E(125°) = 306.79 kcal/mole

E(130°) = 306.03 kcal/mole

E(135°) = 305.41 kcal/mole

E(140°) = 304.94 kcal/mole

E(145°) = 304.61 kcal/mole

E(150°) = 304.38 kcal/mole

E(155°) = 304.25 kcal/mole

E(160°) = 304.17 kcal/mole

E(165°) = 304.12 kcal/mole

E(170°) = 304.08 kcal/mole

E(175°) = 304.01 kcal/mole

Dihedral Driver computing finished successfully

Calculation completed

References

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