

Supporting Information

**Highly Syndiotactic or Isotactic Polyhydroxyalkanoates by
Ligand-Controlled Yttrium-Catalyzed Stereoselective Ring-Opening
Polymerization of Functional Racemic β -Lactones**

Romain Ligny, Mikko M. Hänninen, Sophie M. Guillaume, and Jean-François Carpentier**

anie_201704283_sm_miscellaneous_information.pdf

Supporting Information

Contents

General Considerations

Instrumentations and Measurements

Typical carbonylation procedure

Typical polymerization procedure

Computational details

Additional computational discussion

Tables and Figures caption.

Table S1. ROP of *rac*-BPL^{OR} mediated by **1**/*i*PrOH systems in toluene.

Table S2. Kinetic data for monitoring the ROP of *rac*-BPL^{OAll} with various **1**/*i*PrOH (1:1) systems (see Figure S2).

Table S3. ROP of *rac*-BPL^{OR} mediated by **1**/*i*PrOH systems in toluene.

Figure S1. ¹H NMR spectrum (400 MHz, CDCl₃, 25 °C) of *rac*-BPL^{OAll}, *rac*-BPL^{OMe} and *rac*-BPL^{OBn} (▲ stands for residual water from deuterated solvent).

Figure S2. Semi-logarithmic first-order plots for the ROP of *rac*-BPL^{OAll} initiated by **1**/*i*PrOH (1:1) systems (▲, **1g**; ■, **1b**; ●, **1d**; ●, **1c**; ■, **1a**) in 1M toluene solutions at [Y] = 13.1 mM at 23 °C, and (□) with **1b** at [Y] = 3.3 mM (Table S2).

Figure S3. Plot of experimental (symbols, as determined by ¹H NMR analysis) and theoretical (solid line) *M_n* values of PHB^{OAll} obtained from the ROP of *rac*-BPL^{OAll} initiated by **1**/*i*PrOH (1:1) systems (▲, **1g**; ■, **1b**; ●, **1d**; ●, **1c**), as a function of monomer conversion. Reaction conditions: [*rac*-BPL^{OAll}]₀ = 1 M, toluene, 23 °C (Table S2).

Figure S4. ¹H NMR spectrum (500 MHz, CDCl₃, 25 °C) of a *syndiotactic* PHB^{OAll} prepared from the ROP of *rac*-BPL^{OAll} with the **1g**/*i*PrOH (1:1) system (*P_r* = 0.88; Table 1, entry 6).

Figure S5. ¹³C{¹H} NMR spectrum (125 MHz, CDCl₃, 25 °C) of a *syndiotactic* PHB^{OAll} prepared from the ROP of *rac*-BPL^{OAll} with the **1g**/*i*PrOH (1:1) system (*P_r* = 0.88; Table 1, entry 6).

Figure S6. ¹H NMR spectrum (500 MHz, CDCl₃, 25 °C) of a *syndiotactic* PHB^{OMe} prepared from the ROP of *rac*-BPL^{OMe} with the **1g**/*i*PrOH (1:1) system (*P_r* = 0.81; Table 1, entry 10).

Figure S7. ¹³C{¹H} NMR spectrum (125 MHz, CDCl₃, 25 °C) of a *syndiotactic* PHB^{OMe} prepared from the ROP of *rac*-BPL^{OMe} with the **1g**/*i*PrOH (1:1) system (*P_r* = 0.81; Table 1, entry 10).

Figure S8. ¹H NMR spectrum (500 MHz, CDCl₃, 25 °C) of a *syndiotactic* PHB^{OBn} prepared from the ROP of *rac*-BPL^{OBn} with the **1g**/*i*PrOH (1:1) system (*P_r* = 0.88; Table 1, entry 13) (▲ stands for residual pentane).

Figure S9. ¹³C{¹H} NMR spectrum (125 MHz, CDCl₃, 25 °C) of a *syndiotactic* PHB^{OBn} prepared from the ROP of *rac*-BPL^{OBn} with the **1g**/*i*PrOH (1:1) system (*P_r* = 0.88; Table 1, entry 13) (▲ stands for residual pentane).

Figure S10. ESI mass spectrum of a *syndiotactic* PHB^{OAll} prepared from the ROP of *rac*-BPL^{OAll} with the **1g**/*i*PrOH (1:1) system (*P_r* = 0.88; Table 1, entry 6).

Figure S11. Top: ESI mass spectrum of a *syndiotactic* PHB^{OAll} prepared from the ROP of *rac*-BPL^{OAll} with the **1g**/*i*PrOH (1:1) system (*P_r* = 0.88; Table 1, entry 6). Bottom: Simulation of *i*PrO-PHB^{OAll}-H for *n* = 9.

Figure S12. Top: ESI mass spectrum of a *syndiotactic* PHB^{OAll} prepared from the ROP of *rac*-BPL^{OAll} with the **1g**/*i*PrOH (1:1) system (*P_r* = 0.88; Table 1, entry 6) with H₂O fragmentation. Bottom: Simulation of *i*PrO-PHB^{OAll}-CO(CH)₂CH₂OAll for *n* = 9.

Figure S13. Top: ESI mass spectrum of a *syndiotactic* PHB^{OAll} prepared from the ROP of *rac*-BPL^{OAll} with the **1g**/*i*PrOH (1:1) system (*P_r* = 0.88; Table 1, entry 6) with isopropyl fragmentation. Bottom: Simulation of HO-PHB^{OAll}-H for *n* = 9.

Figure S14. Top: ESI mass spectrum of a *syndiotactic* PHB^{OAll} prepared from the ROP of *rac*-BPL^{OAll} with the **1g**/*i*PrOH (1:1) system ($P_r = 0.88$; Table 1, entry 6) with end-chain fragmentation. Bottom: Simulation cyclic PHB^{OAll} for $n = 9$.

Figure S15. ESI mass spectrum of a *syndiotactic* PHB^{OMe} prepared from the ROP of *rac*-BPL^{OMe} with the **1g**/*i*PrOH (1:1) system ($P_r = 0.81$; Table 1, entry 10).

Figure S16. Top: ESI mass spectrum of a *syndiotactic* PHB^{OMe} prepared from the ROP of *rac*-BPL^{OMe} with the **1g**/*i*PrOH (1:1) system ($P_r = 0.88$; Table 1, entry 10). Bottom: Simulation of *i*PrO-PHB^{OMe}-H for $n = 10$.

Figure S17. Top: ESI mass spectrum of a *syndiotactic* PHB^{OMe} prepared from the ROP of *rac*-BPL^{OMe} with the **1g**/*i*PrOH (1:1) system ($P_r = 0.81$; Table 1, entry 10) with H₂O fragmentation. Bottom: Simulation of *i*PrO-PHB^{OMe}-CO(CH)₂CH₂OAll for $n = 10$.

Figure S18. Detailed regions of ¹³C{¹H} NMR spectra (125 MHz, CDCl₃, 23 °C) of PHB^{OMe} prepared from the ROP of *rac*-BPL^{OMe} (except top spectrum, from *enantiopure* (*R*)-BPL^{OMe}) by **1**/*i*PrOH (1:1) systems (Tables 1, S1).

Figure S19. Details of ¹³C{¹H} NMR spectra (125 MHz, CDCl₃, 23 °C) of PHB^{OBn} prepared from the ROP of *rac*-BPL^{OBn} by **1**/*i*PrOH (1:1) systems (Tables 1, S1).

Figure S20. Chiral GLC analysis of *rac*-BPL^{OAll} prepared from the carbonylation of *rac*-glycidyl allyl ether.

Figure S21. Chiral GLC analysis of the crude *rac*-BPL^{OAll} from the ROP BPL^{OAll} with the **1a**/*i*PrOH system (17% monomer conversion after 2 h).

Figure S22. Shortest CH...Cl distances in **III-SS-TS** (left) and **III-SR-TS** (right).

Figure S23. Proposed ROP mechanism and energetics for *isotactic* (black) and *syndiotactic* (red) polymer formation with **1c** as initiator.

Figure S24. DSC thermogram (second heating cycle; heating rate = 10 °C.min⁻¹; from -80 to 140 °C; helium flow) of a *syndiotactic* PHB^{OAll} sample prepared from the ROP of *rac*-BPL^{OAll} with the **1e**/*i*PrOH (1:1) system ($P_r = 0.81$; Table S1, entry 4; Table S3) ($\Delta H_{\text{melt}} = 23.5 \text{ J.g}^{-1}$).

Figure S25. DSC thermogram (second heating cycle; heating rate = 10 °C.min⁻¹; from -80 to 40 °C; helium flow) of a *syndiotactic* PHB^{OMe} prepared from the ROP of *rac*-BPL^{OMe} with the **1g**/*i*PrOH system ($P_r = 0.81$; Table 1, entry 10; Table S3) ($\Delta H_{\text{melt}} = 29.5 \text{ J.g}^{-1}$).

Figure S26. DSC thermogram (second heating cycle; heating rate = 10 °C.min⁻¹; from -80 to 140 °C; helium flow) of a *syndiotactic* PHB^{OBn} sample prepared from the ROP of *rac*-BPL^{OBn} with the **1h**/*i*PrOH system ($P_r = 0.90$; Table 1, entry 14; Table S3).

Figure S27. DSC thermogram (second heating cycle; heating rate = 10 °C.min⁻¹; from -80 to 140 °C; helium flow) of an *isotactic* PHB^{OAll} sample prepared from the ROP of (*S*)-BPL^{OAll} with the **1h**/*i*PrOH (1:1) system ($P_r < 0.05$; Table S1, entry 7; Table S3).

Figure S28. DSC thermogram (second heating cycle; heating rate = 10 °C.min⁻¹; from -80 to 140 °C; helium flow) of an *isotactic* PHB^{OMe} sample prepared from the ROP of (*R*)-BPL^{OMe} with the **1h**/*i*PrOH (1:1) system ($P_r < 0.05$; Table S1, entry 10; Table S3).

Figure S29. DSC thermogram (second heating cycle; heating rate = 10 °C.min⁻¹; from -80 to 140 °C; helium flow) of an *isotactic* PHB^{OBn} sample prepared from the ROP of (*R*)-BPL^{OBn} with the **1h**/*i*PrOH (1:1) system ($P_r < 0.05$; Table S1, entry 15; Table S3).

General Considerations

All manipulations involving organometallic catalysts were performed under inert atmosphere (argon, < 3 ppm O₂) using standard Schlenk, vacuum line, and glovebox techniques. Solvents were freshly distilled from Na/benzophenone under argon and degassed thoroughly by freeze-thaw-vacuum cycles prior to use. Isopropyl alcohol (Acros) was distilled over Mg turnings under argon atmosphere and kept over activated 3–4 Å molecular sieves. CDCl₃ was dried over a mixture of 3 and 4 Å molecular sieves. Bisphenol [ONXO^{R'2}]₂H₂ proligands and yttrium amide precursors **1a-y** were synthesized according to the methods reported in the literature.¹ *Racemic* glycidyl allyl ether, glycidyl benzyl ether, and glycidyl methyl ether were used as received (Sigma). (*S*)-Glycidyl allyl ether, (*R*)-glycidyl allyl ether, (*R*)-glycidyl methyl ether and (*R*)-glycidyl benzyl ether were prepared by hydrolytic kinetic resolution (HKR) of the corresponding *racemic* compound following the reported procedure.² Salph(Cr(THF)₂)[Co(CO)₄],^{3,4} *racemic* 4-allyloxymethyl-β-propiolactone (*rac*-BPL^{OAll}),⁵ 4-(*S*)-allyloxymethyl-β-propiolactone ((*S*)-BPL^{OAll}), 4-(*R*)-allyloxymethyl-β-propiolactone ((*R*)-BPL^{OAll}), *racemic* 4-methyloxymethyl-β-propiolactone (*rac*-BPL^{OMe}),⁵ 4-(*R*)-methyloxymethyl-β-propiolactone ((*R*)-BPL^{OMe}),⁵ *racemic* 4-benzyloxymethyl-β-propiolactone (*rac*-BPL^{OBn}),⁵ and 4-(*R*)-benzyloxymethyl-β-propiolactone ((*R*)-BPL^{OBn})⁵ were synthesized according to the literature procedure, respectively.

Instrumentation and measurements

¹H (500 and 400 MHz) and ¹³C{¹H} (125 MHz) NMR spectra were recorded on Bruker Avance AM 500 and Ascend 400 spectrometers at 25 °C. ¹H and ¹³C{¹H} NMR spectra were referenced internally relative to SiMe₄ (δ 0 ppm) using the residual solvent resonances.

Average molar mass ($M_{n,SEC}$) and dispersity ($D_M = M_w / M_n$) values of the PHB^{ORs} were determined by size-exclusion chromatography (SEC) in THF at 30 °C (flow rate = 1.0 mL.min⁻¹) on a Polymer Laboratories PL50 apparatus equipped with a refractive index detector and a set of two ResiPore PLgel 3 μm MIXED-D 300 × 7.5 mm columns. The polymer samples were dissolved in THF (2 mg.mL⁻¹). All elution curves were calibrated with polystyrene standards; $M_{n,SEC}$ values of the PHB^{ORs} were uncorrected for the possible difference in hydrodynamic radius vs. that of polystyrene.

The molar masses of PHB^{ORs} samples were determined also by ¹H NMR analysis in CDCl₃ from the relative intensities of the signals of the PHB^{OAll} main-chain methine hydrogens (–OCH(CH₂OAll)CH₂, δ 5.50 ppm), PHB^{OMe} main-chain methine (–OCH(CH₂OMe)CH₂, δ 5.33 ppm), PHB^{OBn} main-chain methine (–OCH(CH₂OBn)CH₂, δ 5.38 ppm) and those of the chain-end isopropyl (–OCH(CH₃)₂, δ 1.21 ppm).

Monomer conversions were calculated from ¹H NMR spectra of the crude polymer samples in CDCl₃ by using the integration (Int.) ratio Int._{PHBOR}/[Int._{PHBOR} + Int._{BPLOR}] of the methine hydrogens (δ 4.65 ppm for BPL^{OAll}, δ 4.63 ppm for BPL^{OMe} and δ 4.63 ppm for BPL^{OBn}).

Chiral GLC analysis of BPL^{OAll} was performed on a Shimadzu chromatograph equipped with a capillary Chiralcel-OD (25 m × 0.2 mm) column at 135 °C (constant temperature), using helium as carrier gas (0.94 mL.min⁻¹, pressure: 101 kPa).

Typical carbonylation procedure⁵

Carbonylation of racemic allyl glycidyl ether (G^{OAll}) to rac-BPL^{OAll}. In a typical experiment, in the glovebox, a Schlenk flask was charged with [Salph(Cr(THF)₂)] [Co(CO)₄] (320 mg, 0.35 mmol). On a vacuum line, dry DME (15 mL) was syringed in and the resulting

solution was cannulated into a degassed high pressure reactor which was pressurized with carbon monoxide to 20 bar, and stirred for 15 min before depressurization. A solution of *racemic* allyl glycidyl ether (G^{OAll}) (3.93 g, 34.5 mmol, 100 equiv.) in dry DME (15 mL) was transferred into the reactor which was then pressurized with CO to 30 bar. The reaction mixture was stirred for 3 days at 20 °C. Then, the reactor was vented to atmospheric pressure, volatiles were removed under vacuum and the crude product was purified through a short alumina column ($CHCl_3$, 2×200 mL). After evaporation of volatiles, *rac*-BPL^{OAll} was obtained by double distillation using a Kügelrohr oven (110 °C–130 °C, 0.1 torr) to afford a colorless viscous liquid (79%). ¹H NMR (400 MHz, $CDCl_3$, 25 °C): δ (ppm): 3.43 (m, 2H), 3.73 (m, 2H), 4.05 (m, 2H), 4.64 (m, 1H), 5.24 (m, 2H), 5.87 (m, 1H) (Figure S1). ¹³C NMR (125 MHz, $CDCl_3$, 25 °C) δ (ppm): 39.7 ($CH_2C(O)O$), 69.3 ($OCH_2CH=CH_2$), 69.5 ($CHOC(O)$), 72.7 (CH_2OAll), 117.7 ($OCH_2CH=CH_2$), 134.1 ($OCH_2CH=CH_2$), 167.9 ($C=O$). The carbonylation of (*S*)-glycidyl allyl ether and (*R*)-glycidyl allyl ether was performed similarly and gave (*S*)-BPL^{OAll} as a colorless viscous liquid in 31% yield and (*R*)-BPL^{OAll} as a colorless viscous liquid in 74% yield; NMR characteristics are identical to those of *rac*-BPL^{OAll}.

*Carbonylation of racemic glycidyl methyl ether (G^{OMe}) to *rac*-BPL^{OMe}.* Following the aforementioned typical procedure, starting from [Salph(Cr(THF)₂)] [Co(CO)₄] (403 mg, 0.44 mmol) and *rac*- G^{OMe} (3.20 g, 43.3 mmol, 100 equiv), *rac*-BPL^{OMe} was isolated as a colorless viscous liquid (51% yield). ¹H NMR (400 MHz, $CDCl_3$, 25 °C) δ (ppm): 3.40 (m, 2H), 3.42 (s, 3H), 3.67 (m, 2H), 4.63 (m, 1H) (Figure S1). ¹³C NMR (125 MHz, $CDCl_3$, 25 °C) δ (ppm): 39.7 ($CH_2C(O)O$), 59.8 (OCH_3), 69.6 ($CHOC(O)$), 72.1 (CH_2OCH_3), 167.9 ($C=O$). The carbonylation of (*S*)-glycidyl methyl ether was performed similarly and yielded (*S*)-

BPL^{OMe} as a colorless viscous liquid in 70% yield; NMR characteristics are identical to those of *rac*-BPL^{OMe}.

Carbonylation of racemic glycidyl benzyl ether (G^{OBn}) to rac-BPL^{OBn}. Following the typical experiment reported above, using [Salph(Cr(THF)₂)]Co(CO)₄ (246 mg, 0.27 mmol) and *rac*-G^{OBn} (4.43 g, 27.0 mmol, 100 equiv), *rac*-BPL^{OBn} was isolated as a colorless viscous liquid (58% yield). ¹H NMR (400 MHz, CDCl₃, 25 °C) δ (ppm): 3.42 (m, 2H), 3.75 (s, 2H), 4.60 (m, 2H), 7.34 (m, 5H) (Figure S1). ¹³C NMR (125 MHz, CDCl₃, 25 °C) δ (ppm): 39.7 (CH₂C(O)O), 69.2 (CH₂Ph), 69.3 (CHOC(O)), 73.6 (CH₂OPh), 127.7 (*o*-CH aro), 127.9 (*p*-CH aro), 128.5 (*m*-CH aro), 137.3 (*ipso*-CH aro), 167.6 (C=O). Carbonylation of (*R*)-glycidyl benzyl ether was performed similarly and gave (*R*)-BPL^{OBn} as a colorless viscous liquid in 80% yield; NMR characteristics are identical to those of *rac*-BPL^{OBn}.

Typical polymerization procedure

In a typical experiment, in the glovebox, a Schlenk flask was charged with [Y(N(SiHMe₂)₂)₃](THF)₂ (4.1 mg, 6.5 mmol) and {ONOO^{Cl2}} (2.8 mg, 6.5 mmol), and toluene (0.25 mL) was next added. To this solution, *i*PrOH (50 μL of a 1% (*v/v*) solution in toluene, 6.5 mmol, 1 equiv *vs.* Y) was added under stirring at room temperature. After 5 min of stirring, a solution of *rac*-BPL^{All} (51 mg, 0.33 mmol, 50 equiv) in toluene (0.25 mL) was added rapidly and the mixture was stirred at 20 °C for 2 h. The reaction was quenched by addition of acetic acid (*ca.* 0.5 mL of a 1.6 mol·L⁻¹ solution in toluene). The resulting mixture was concentrated to dryness under vacuum and the conversion was determined by ¹H NMR analysis of the residue in CDCl₃. The crude polymer was then dissolved in CH₂Cl₂ (*ca.* 1 mL) and precipitated in cold pentane (*ca.* 5 mL), filtered and dried. The final polymer was

then analyzed by NMR (Figures S4–S9), ESI MS (Figures S10–S17), SEC, and DSC (Figures S24–S29) analyses.

Computational details

All calculations were performed using Orca 3.0.3 program package.⁶ Geometries were optimized using pure Perdew-Burke-Erzerhoff (PBE) GGA functional⁷ with RI-J approximation as implemented in Orca. Def2-SVP basis set was assigned for all atoms other than yttrium for which larger def2-TZVP basis set with Stuttgart-Dresden effective core potential was used.⁸ Corresponding auxiliary basis sets (def2-SVP/J and def2-TZVP/J) were used for RI approximation.⁹ Full vibrational analysis was performed for all optimized structures to confirm that they represent either a local minimum or a saddle point corresponding to desired transition state.

Additional computational discussion

We began our investigation from intermediate **I-S** which is the result from ring-opening of the first (*S*)-BPL^{O^{All}} monomer. The κ^2 -coordinated polymer ligand is bound to the yttrium center through carbonyl and alkoxide oxygens forming a six-membered metallacycle. This compound can be also seen as a resting state of the catalyst. Attack of next (*S*)- or (*R*)-BPLO^{All} monomer to **I-S** is a slightly exergonic but highly exothermic reaction (Figure 2) forming **II-SS** or **II-SR** intermediates, respectively. It should be noted that the monomer attack can occur from various positions in front (opposite of the ligand cap) or backside of the {ONXO^{R²}}²⁻ ligand but our initial calculations suggested that the selected frontside addition would lead to most energetically favorable geometries. Furthermore, a study by Thomas and Maron *et al.* pointed out that the activation energies between so-called front and backside attacks are almost indistinguishable.¹⁰

Next step in the ROP reaction is the (nucleophilic) addition of the carbonyl carbon of the attacking monomer to the alkoxide oxygen forming intermediate **III-SS/SR** with κ^3 -bound polymeric ligand. Ether oxygen of the BPL^{OAll} monomer will then bend toward the metal center triggering the C–O_{ether} bond dissociation to form intermediate **IV-SS/SR** through transition state **III-SS/SR-TS** and completing the ring opening of the monomer. Finally, detachment of carbonyl oxygen (of the first monomer) from the yttrium and rotation of the polymeric ligand will eventually lead to the intermediate/resting state **V-SS/SR** with almost identical coordination environment to **I**, thus completing the catalytic cycle. The overall ΔG for the complete reaction is $-4.6 \text{ kcal mol}^{-1}$ for (*S,S*)- and $-6.2 \text{ kcal mol}^{-1}$ for (*S,R*)-configuration (Figure S23).

The activation energy of **III-SS-TS** leading to *isotactic* polymer is notably lower compared to **III-SR-TS** (leading to *syndiotactic* polymer). This is hypothesized to be due to the stabilization of the transition state by C–H \cdots Cl interactions. The closest C–H \cdots Cl distance between the alkoxy methylene proton ($-\text{CHCH}_2\text{OCH}_2\text{CH}=\text{CH}_2$) and adjacent chloride in **III-SS-TS** is 2.556 Å (Figure S22) which is markedly shorter than combined Van der Waals radii of the two elements (3.089 Å).¹¹ Furthermore, there exist also another stabilizing close contact (3.083 Å) from the allyl methylene ($-\text{CHCH}_2\text{OCH}_2\text{CH}=\text{CH}_2$) to the chloride substituent. These above interactions are negligible in **III-SR-TS** because the different orientation of the whole alkoxy methylene tail of the BPL^{OAll} monomer. Shortest C–H \cdots Cl distance (3.195 Å) in **III-SR-TS** is from the methine proton ($-\text{CHCH}_2\text{OCH}_2\text{CH}=\text{CH}_2$) to aromatic chloride (Figure S22).

We have performed calculations for **1c** as initiator and the initial results suggest that the ROP reaction occurs through a similar route but with only a minor activation energy difference between *syndio*- and *isoselective* routes ($0.2 \text{ kcal mol}^{-1}$) (Figure S23). At this point

we have located all intermediates but one transition state from the reaction route (**IV-SR-TS**). However, we have found a structure that is barely a minimum (lowest vibration around 4 cm^{-1}) that has similar energetics than **IV-SS-TS**; hence the values from this calculation are used in Figure S23. We are currently performing more elaborate computational analyses considering different, solvent effects and possible alternative mechanisms. This study will be published in due time within the subsequent full paper concerning this work.

References

- ¹ M. Bouyahyi, N. Ajellal, E. Kirillov, C. M. Thomas and J.-F. Carpentier, *Chem. Eur. J.*, **2011**, *17*, 1872-1883.
- ² S. E. Schaus, B. D. Brandes, J. F. Larrow, M. Tokunaga, K. B. Hanse, A. E. Gould, M. E. Furrow, E. N. Jacobsen *J. Am. Chem. Soc.* **2002**, *124*, 1307-1315.
- ³ W. F. Edgell, J. Lyford *Inorg. Chem.* **1970**, *9*, 1932-1933.
- ⁴ J. Wöltinger, J. E. Bäckvall, A. Zsigmond *Chem. Eur. J.* **1999**, *5*, No. 5, 1460-1467.
- ⁵ J. A. R. Schmidt, E. B. Lobkovsky, G. W. Coates, *J. Am. Chem. Soc.* **2005**, *127*, 11426-11435.
- ⁶ Neese, F. The ORCA program system, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.* **2012**, *2*, 73-78.
- ⁷ (a) J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* **1996**, *77*, 3865-3868; (b) J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* **1997**, *78*, 1396-1396.
- ⁸ (a) A. Schaefer, H. Horn and R. Ahlrichs, *J. Chem. Phys.* **1992**, *97*, 2571-2577. (b) A. Schaefer, C. Huber and R. Ahlrichs, *J. Chem. Phys.* **1994**, *100*, 5829-5835. (c) Weigend, F.; Häser, M.; Patzelt, H.; Ahlrichs, R., *Chem. Phys. Lett.* **1998**, *294* (1-3), 143-152; (d) F. Weigend, R. Ahlrichs, *PCCP* **2005**, *7*, 3297-3305.; (e) D. Andrae, U. Haeussermann, M. Dolg, H. Stoll, H. Preuss, *Theor. Chim. Acta*, **1990**, *77*, 123-141.
- ⁹ F. Weigend; *Phys. Chem. Chem. Phys.* **2006**, *8*, 1057-1065.
- ¹⁰ J. Fang, M. J. L. Tschan, T. Roisnel, X. Trivelli, R. M. Gauvin, C. M. Thomas, L. Maron, *Polym. Chem.* **2013**, *4*, 360-367.
- ¹¹ S. Alvarez, *Dalton Trans.* **2013**, *42*, 8617-8636.

Table S1. ROP of *rac*-BPL^{OR} mediated by **1**/*i*PrOH systems in toluene.

Entry	BPL ^{OR}	Cat.	Temp. (°C)	[BPL ^{OR}] ₀ /[1] ₀ /[ROH] ₀ ^a	Time (h) ^b	Conv. (%) ^c	<i>M</i> _{n,theo} ^d (g.mol ⁻¹)	<i>M</i> _{n,NMR} ^e (g.mol ⁻¹)	<i>M</i> _{n,SEC} ^f (g.mol ⁻¹)	<i>D</i> _M ^f	<i>P</i> _r ^g
1	OAll	1a	20	53:1:1	2	15	7 550	nd ^h	nd ^h	nd ^h	nd ^h
2	OAll	1a	60	53:1:1	72	74	7 550	7 150	9 200	1.46	0.07
3	OAll	1b	20	54:1:1	2	94	7 800	7 850	10 500	1.09	0.10
4	OAll	1b	20	68:1:1	2	95	9 700	9 700	14 500	1.09	0.09
5	OAll	1b	60	50:1:1	4	100	7 200	8 500	11 200	1.30	0.13
6	OAll	1c	20	54:1:1	2	39	3 050	3 300	4 300	1.12	0.49
7	OAll	1d	20	50:1:1	2	74	5 300	5 600	7 200	1.11	0.51
8	OAll	1e	20	51:1:1	2	100	7 250	7 250	11 300	1.16	0.76
9	OAll	1e	20	83:1:1	2	100	17 150	17 300	15 950	1.24	0.81
10	OAll	1f	20	53:1:1	2	100	7 550	7 100	9 050	1.19	0.81
11	OAll	1f	20	87:1:1	2	100	12 400	12 450	16 750	1.10	0.83
12	OAll	1g	20	55:1:1	2	100	7 850	7 650	11 000	1.19	0.88
13	OAll	1g	0	51:1:1	2	100	7 250	7 950	12 150	1.39	0.91
14	OAll	1g	20	108:1:1	2	100	15 290	15 150	18 300	1.14	0.84
15	OAll	1h	20	53:1:1	2	100	7 500	7 450	8 600	1.23	0.82
16	(<i>S</i>)-OAll	1h	20	51:1:1	2	100	7 500	6 500	7 300	1.06	<0.05
17	OMe	1a	20	47:1:1	2	traces	5 500	nd ^h	nd ^h	nd ^h	nd ^h
18	OMe	1b	20	44:1:1	2	84	4 350	5 200	5 200	1.06	0.10
19	OMe	1e	20	50:1:1	2	100	5 900	6 100	6 950	1.09	0.78
20	OMe	1f	20	61:1:1	2	100	6 300	6 250	5 500	1.06	0.79
21	OMe	1g	20	49:1:1	2	100	5 750	5 750	8 400	1.18	0.81
22	OMe	1h	20	43:1:1	2	100	5 050	4 950	6 850	1.07	0.78
23	(<i>R</i>)-OMe	1h	20	48:1:1	2	100	5 200	3 500	5 600	1.08	<0.05
24	OBn	1a	20	53:1:1	2	15	1 400	nd ^h	nd ^h	nd ^h	nd ^h
25	OBn	1b	20	47:1:1	2	98	9 100	11 550	11 000	1.08	0.10
26	OBn	1e	20	52:1:1	2	100	10 000	10 200	11 300	1.13	0.85
27	OBn	1f	20	52:1:1	2	100	10 000	10 200	9 600	1.09	0.86
28	OBn	1g	20	52:1:1	2	100	10 000	11 400	16 400	1.14	0.88
29	OBn	1h	20	51:1:1	2	100	9 850	10 050	10 500	1.07	0.90
30	(<i>R</i>)-OBn	1h	20	53:1:1	2	100	9 500	7 400	10 200	1.06	<0.05

^a Reactions performed at [BPL^{OR}]₀ = 1.0 M. ^b Reaction time was not necessarily optimized. ^c Conversion of BPL^{OR} as determined by ¹H NMR analysis of the crude reaction mixture. ^d Molar mass calculated according to *M*_{n,theo} = ([BPL^{OR}]₀/[**1**]₀ × conv._{BPLOR} × *M*_{BPLOR}) + *M*_{PrOH}, with *M*_{BPLOR} = 142 g.mol⁻¹, *M*_{PrOH} = 60 g.mol⁻¹. ^e Molar mass determined by ¹H NMR analysis of the isolated polymer, from resonances of the terminal O/Pr group. ^f Number-average molar mass and dispersity (*M*_w/*M*_n) determined by SEC analysis in THF at 30 °C vs. polystyrene standards (uncorrected values). ^g *P*_r is the probability of *racemic* linkages between BPL^{OR} units as determined by ¹³C{¹H} NMR analysis of the isolated PHB^{OR}s. ^h not determined.

Table S2. Kinetic data for monitoring the ROP of *rac*-BPL^{OAll} with various **1**/*i*PrOH (1:1) systems (see Figure S2).

(cat = 1b) [Y] = 13.1 mM		n(BPL^{OAll})₀ (μmol)						
			951					
t (min)	conv. (%)	n(BPL ^{OAll})(t)	ln([BPL ^{OAll}] ₀ /[BPL ^{OAll}] _t)	<i>M</i> _{n,SEC}	<i>M</i> _{n,NMR}	<i>M</i> _{n,theo}		
0	0	0	0	0	0	59		
35	0.55	428	0.80	7 500	4 400	3 800		
60	0.77	221	1.46	10 350	5 900	5 300		
90	0.88	112	2.14	11 100	6 800	6 100		

(cat = 1a) [Y] = 13.1 mM		n(BPL^{OAll})₀ (μmol)						
			1050					
t (min)	conv. (%)	n(BPL ^{OAll})(t)	ln([BPL ^{OAll}] ₀ /[BPL ^{OAll}] _t)					
0	0	1050	0					
35	0.03	1018	0.03					
60	0.06	987	0.06					
90	0.09	956	0.09					

(cat = 1d) [Y] = 13.1 mM		n(BPL^{OAll})₀ (μmol)						
			946					
t (min)	conv. (%)	n(BPL ^{OAll})(t)	ln([BPL ^{OAll}] ₀ /[BPL ^{OAll}] _t)	<i>M</i> _{n,SEC}	<i>M</i> _{n,NMR}	<i>M</i> _{n,theo}		
0	0	0	0	0	0	59		
35	0.37	596	0.46	4 500	2 400	2 600		
60	0.50	473	0.69	5900	3 200	3 500		
90	0.59	388	0,89	6 700	3 700	4 100		

(cat = 1c) [Y] = 13.1 mM		n(BPL^{OAll})₀ (μmol)						
			974					
t (min)	conv. (%)	n(BPL ^{OAll})(t)	ln([BPL ^{OAll}] ₀ /[BPL ^{OAll}] _t)	<i>M</i> _{n,SEC}	<i>M</i> _{n,NMR}	<i>M</i> _{n,theo}		
0	0	0	0	0	0	59		
35	0.19	792	0.21	2 300	1 500	1 400		
60	0.32	663	0.39	3 400	2 400	2 300		
90	0.42	563	0.55	4 200	2 900	3 000		

(cat = 1g) [Y] = 13.1 mM		n(BPL^{OAll})₀ (μmol)						
			1726					
t (min)	conv. (%)	n(BPL ^{OAll})(t)	ln([BPL ^{OAll}] ₀ /[BPL ^{OAll}] _t)	<i>M</i> _{n,SEC}	<i>M</i> _{n,NMR}	<i>M</i> _{n,theo}		
0,00	0	0	0	0	0	59		
0.50	0.71	489	1.25	7 100	8 500	5 500		
0.83	0.89	187	2.21	8 100	8 600	6 300		
1.17	0.95	84	3.01	8 600	9 500	7 200		
1.50	0.97	58	3.39	9 600	9 600	7 400		

(cat = 1b) [Y] = 3.3 mM		$[\text{BPL}^{\text{OAll}}]_0$ (μmol)				
			339			
t (min)	conv. (%)	n(BPL^{OAll})(t)	$\ln([\text{BPL}^{\text{OAll}}]_0/[\text{BPL}^{\text{OAll}}]_t)$	$M_{n,\text{NMR}}$	$M_{n,\text{theo}}$	
0	0.00	339	0	0	0	
15	0.25	253	0.29	3 000	1 900	
29	0.36	216	0.45	3 400	2 700	
45	0.44	188	0.59	3 600	3 300	
60	0.50	169	0.69	4 000	3 800	
90	0.60	137	0.91	4 800	4 500	
118	0.66	117	1.06	5 000	4 900	
180	0.85	51	1.90	6 400	6 300	
300	0.91	31	2.43	7 000	6 800	

Table S3. ROP of *rac*-BPL^{OR} mediated by **1**/*i*PrOH systems in toluene.

BPL ^{OR}	Cat.	P_r	T_g^a (°C)	T_m^a (°C)	T_c^a (°C)
OAll	1g	0.88	-36	85 (26.8 J/g)	46
OAll	1e	0.81	-36	72 (23.5 J/g)	10
OAll	1b	0.09	-42	no ^b	no ^b
(<i>S</i>)-OAll	1g	<0.05	-39	no ^b	no ^b
OMe	1g	0.81	-11	117	61
OMe	1b	0.10	-12	no ^b	no ^b
(<i>R</i>)-OMe	1g	<0.05	-18	no ^b	no ^b
OBn	1h	0.90	0	no ^b	no ^b
OBn	1g	0.88	0	no ^b	no ^b
OBn	1b	0.10	-1	no ^b	no ^b
(<i>R</i>)-OBn	1g	<0.05	0	no ^b	no ^b

^a Glass, melting and crystallization transition temperature as determined by differential scanning calorimetry (DSC). ^b Not observed.

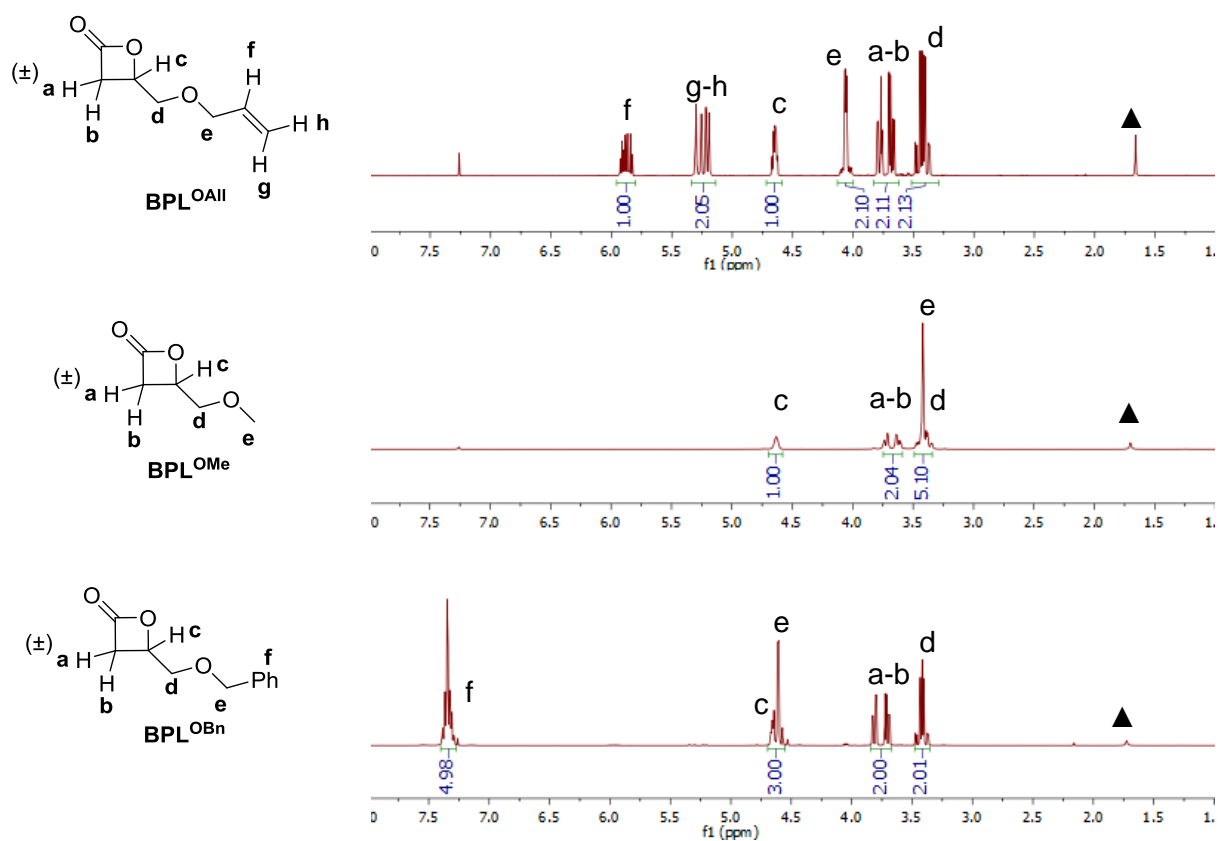


Figure S1. ^1H NMR spectrum (400 MHz, CDCl_3 , 25 $^\circ\text{C}$) of *rac*-BPL^{OAll}, *rac*-BPL^{OMe} and *rac*-BPL^{OBn} (\blacktriangle stands for residual water from deuterated solvent).

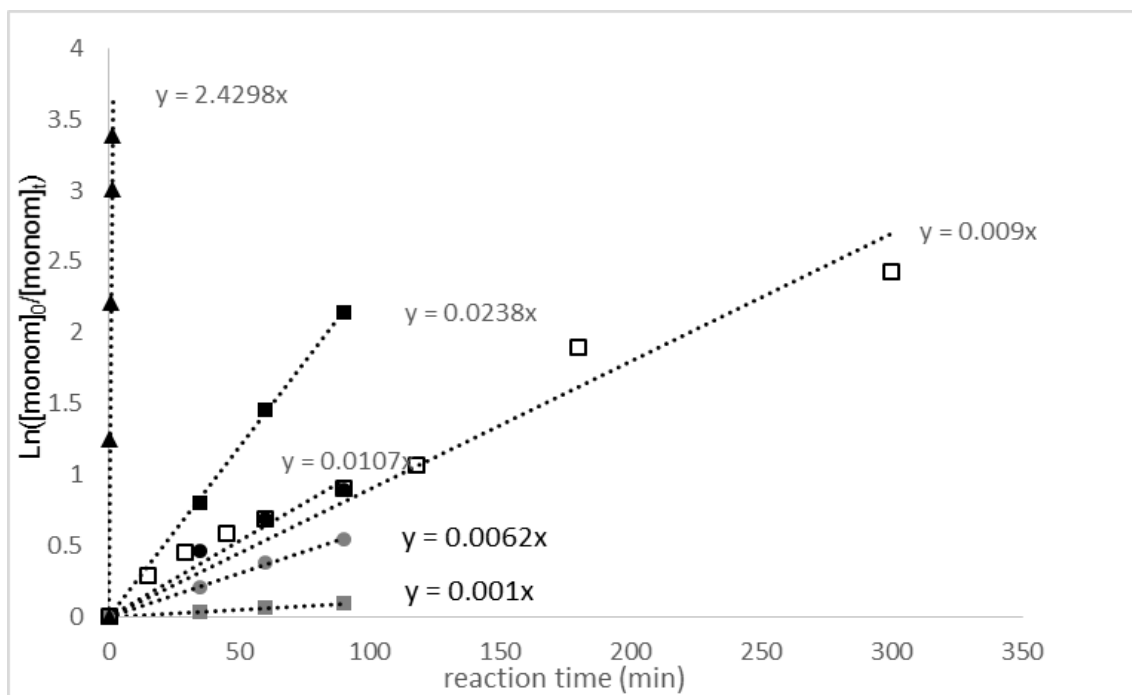


Figure S2. Semi-logarithmic first-order plots for the ROP of $rac\text{-BPL}^{\text{OAll}}$ initiated by 1/*i*PrOH (1:1) systems (▲, **1g**; ■, **1b**; ●, **1d**; ●, **1c**; ■, **1a**) in 1M toluene solutions at [Y] = 13.1 mM at 23 °C, and (□) with **1b** at [Y] = 3.3 mM (Table S2).

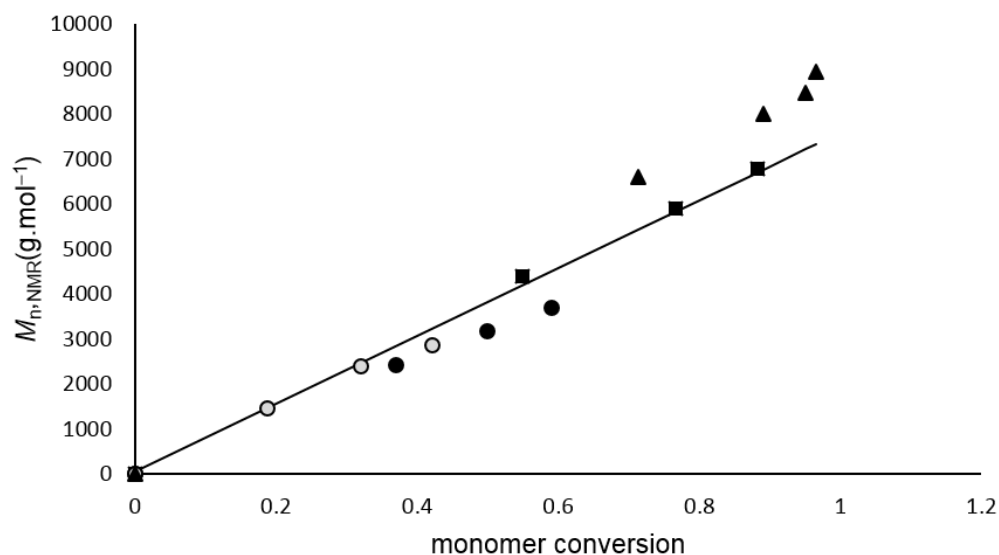


Figure S3. Plot of experimental (symbols, as determined by ^1H NMR analysis) and theoretical (solid line) M_n values of PHB^{OAll} obtained from the ROP of $rac\text{-BPL}^{\text{OAll}}$ initiated by 1/*i*PrOH (1:1) systems (▲, **1g**; ■, **1b**; ●, **1d**; ●, **1c**), as a function of monomer conversion. Reaction conditions: $[rac\text{-BPL}^{\text{OAll}}]_0 = 1 \text{ M}$, toluene, 23 °C (Table S2).

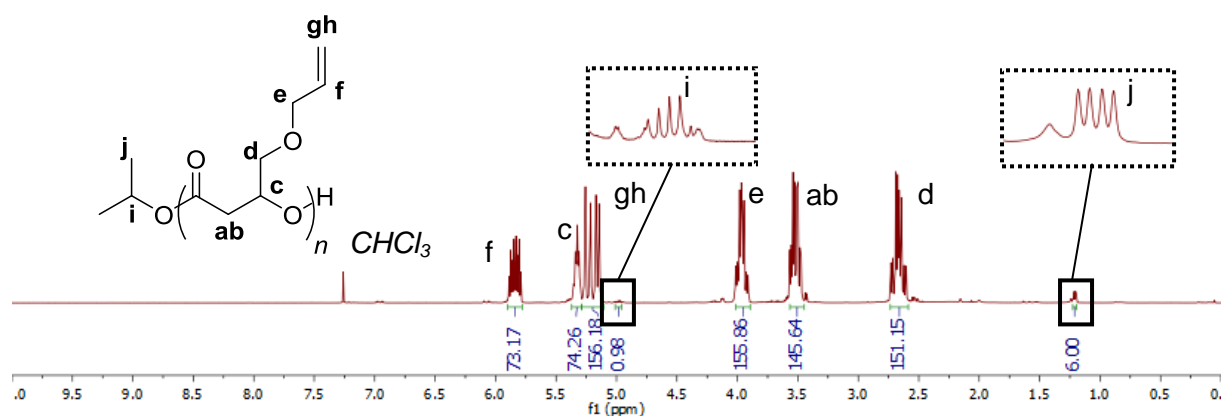


Figure S4. ¹H NMR spectrum (500 MHz, CDCl₃, 25 °C) of a syndiotactic PHB^{OAll} prepared from the ROP of *rac*-BPL^{OAll} with the **1g**/*i*PrOH (1:1) system ($P_r = 0.88$; Table 1, entry 6).

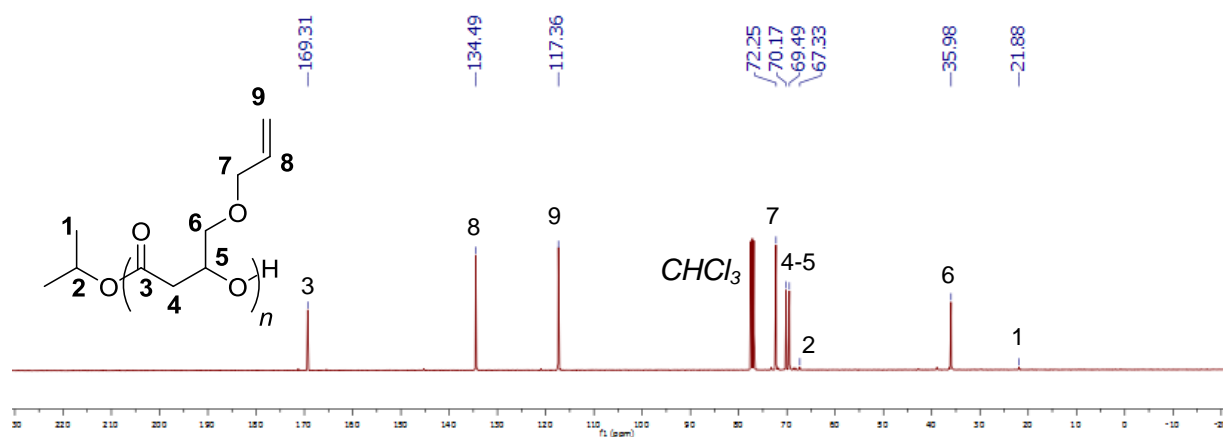


Figure S5. ¹³C{¹H} NMR spectrum (125 MHz, CDCl₃, 25 °C) of a syndiotactic PHB^{OAll} prepared from the ROP of *rac*-BPL^{OAll} with the **1g**/*i*PrOH (1:1) system ($P_r = 0.88$; Table 1, entry 6).

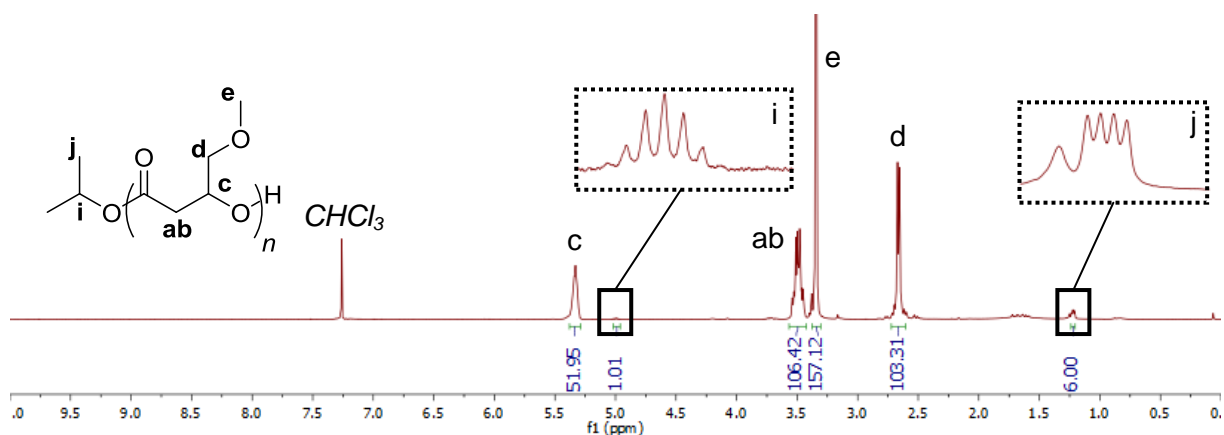


Figure S6. ^1H NMR spectrum (500 MHz, CDCl_3 , 25 °C) of a syndiotactic PHB^{OMe} prepared from the ROP of $\text{rac-BPL}^{\text{OMe}}$ with the **1g**/*i*PrOH (1:1) system ($P_r = 0.81$; Table 1, entry 10).

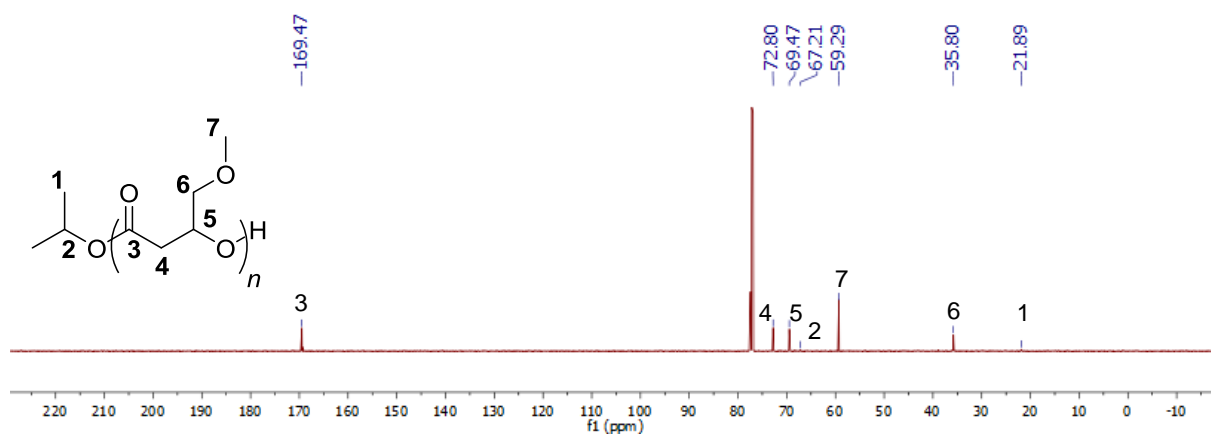


Figure S7. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3 , 25 °C) of a syndiotactic PHB^{OMe} prepared from the ROP of $\text{rac-BPL}^{\text{OMe}}$ with the **1g**/*i*PrOH (1:1) system ($P_r = 0.81$; Table 1, entry 10).

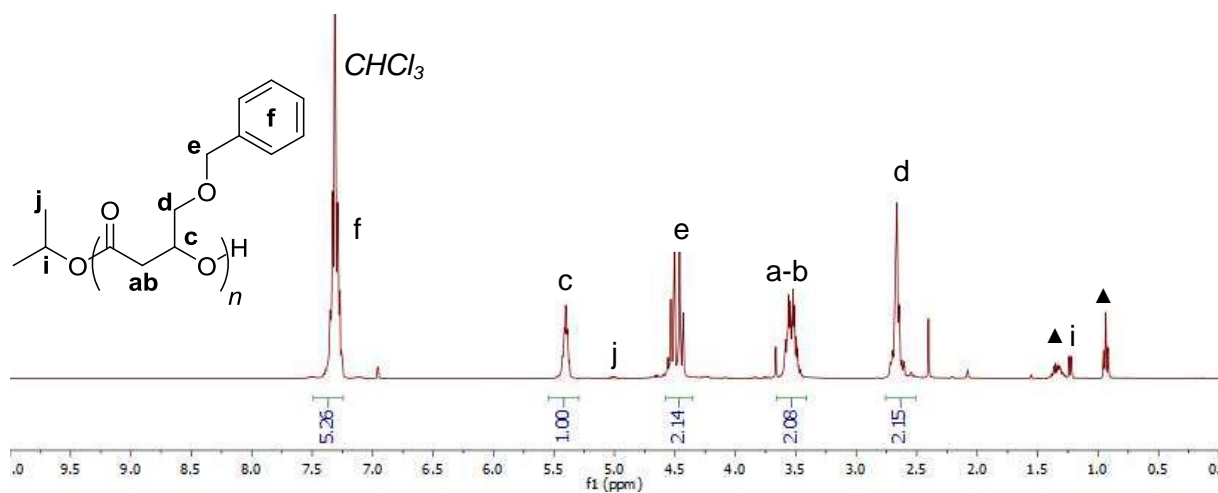


Figure S8. ^1H NMR spectrum (500 MHz, CDCl_3 , 25 °C) of a syndiotactic PHB^{OBn} prepared from the ROP of $\text{rac-BPL}^{\text{OBn}}$ with the **1g**/*i*PrOH (1:1) system ($P_r = 0.88$; Table 1, entry 13) (▲ stands for residual pentane).

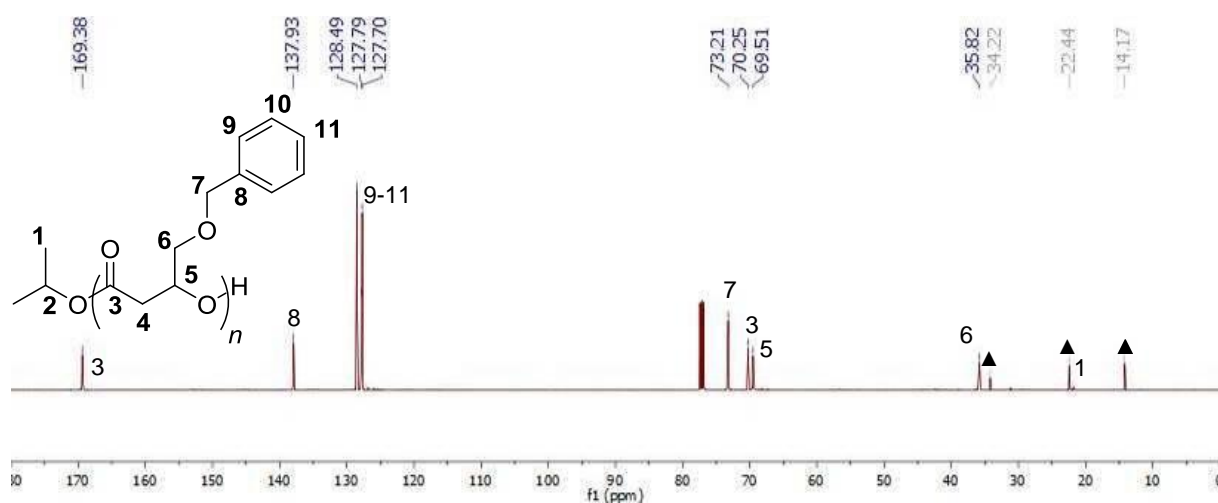


Figure S9. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (125 MHz, CDCl_3 , 25 °C) of a PHB^{OBn} prepared from the ROP of $\text{rac-BPL}^{\text{OBn}}$ with the **1g**/*i*PrOH (1:1) system ($P_r = 0.88$; Table 1, entry 13) (▲ stands for residual pentane).

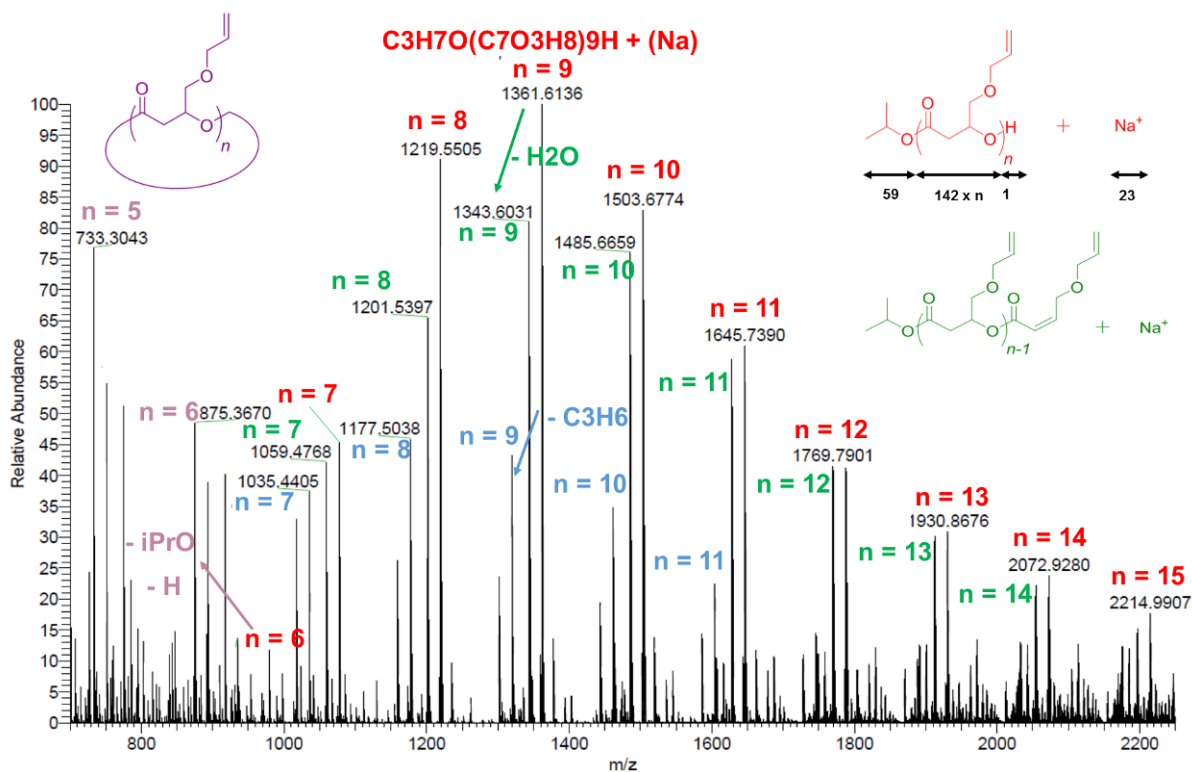


Figure S10. ESI mass spectrum of a *syndiotactic* PHB^{OAll} prepared from the ROP of *rac*-BPL^{OAll} with the **1g**/*i*PrOH (1:1) system ($P_r = 0.88$; Table 1, entry 6). The major population corresponds to *i*PrO-PHB^{OAll}-H macromolecules ionized by Na⁺, the second corresponds to the loss of water and the third to the fragmentation of isopropyl.

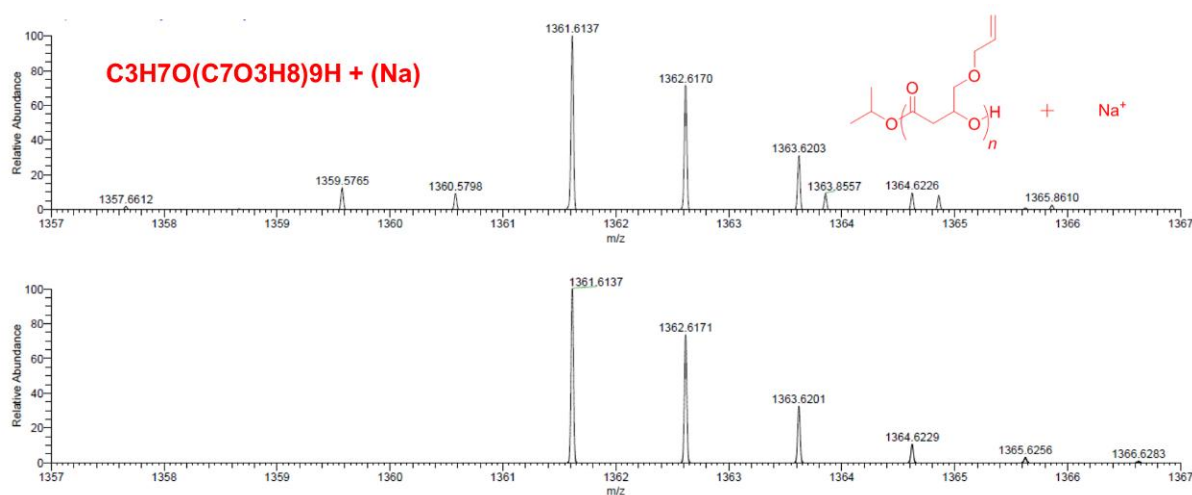


Figure S11. Top: ESI mass spectrum of a *syndiotactic* PHB^{OAll} prepared from the ROP of *rac*-BPL^{OAll} with the **1g**/*i*PrOH (1:1) system ($P_r = 0.88$; Table 1, entry 6). Bottom: Simulation of *i*PrO-PHB^{OAll}-H for $n = 9$.

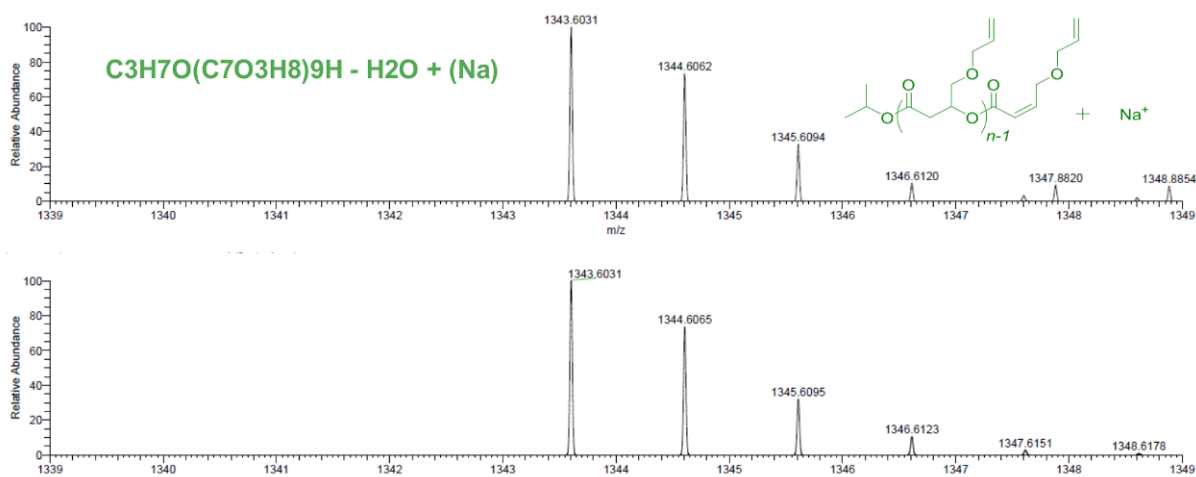


Figure S12. Top: ESI mass spectrum of a *syndiotactic* PHB^{OAll} prepared from the ROP of *rac*-BPL^{OAll} with the **1g**/*i*PrOH (1:1) system ($P_r = 0.88$; Table 1, entry 6) with H₂O fragmentation. Bottom: Simulation of *i*PrO-PHB^{OAll}-CO(CH₂)₂CH₂OAll for $n = 9$.

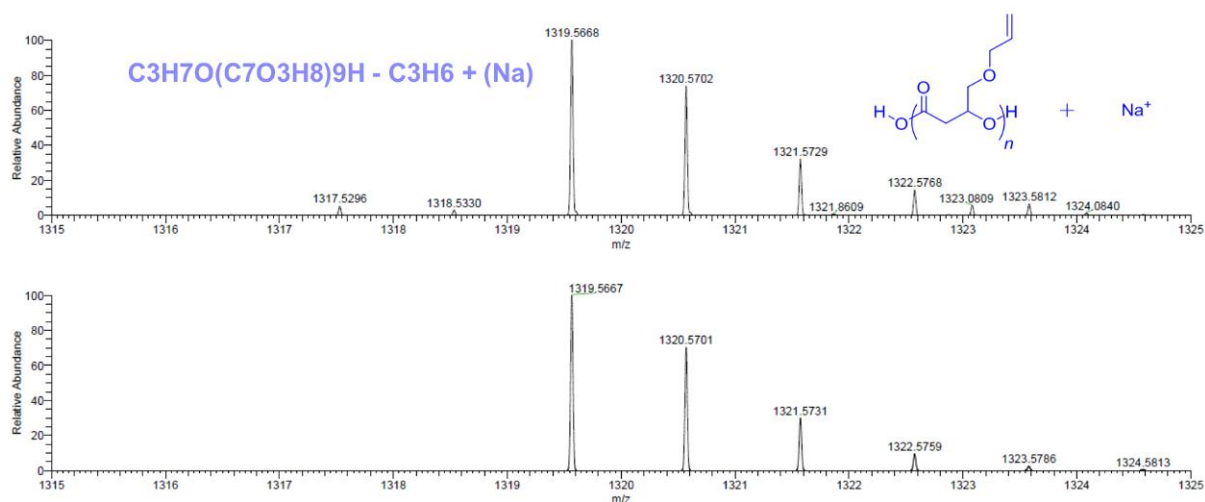


Figure S13. Top: ESI mass spectrum of a *syndiotactic* PHB^{OAll} prepared from the ROP of *rac*-BPL^{OAll} with the **1g**/*i*PrOH (1:1) system ($P_r = 0.88$; Table 1, entry 6) with isopropyl fragmentation. Bottom: Simulation of HO-PHB^{OAll}-H for $n = 9$.

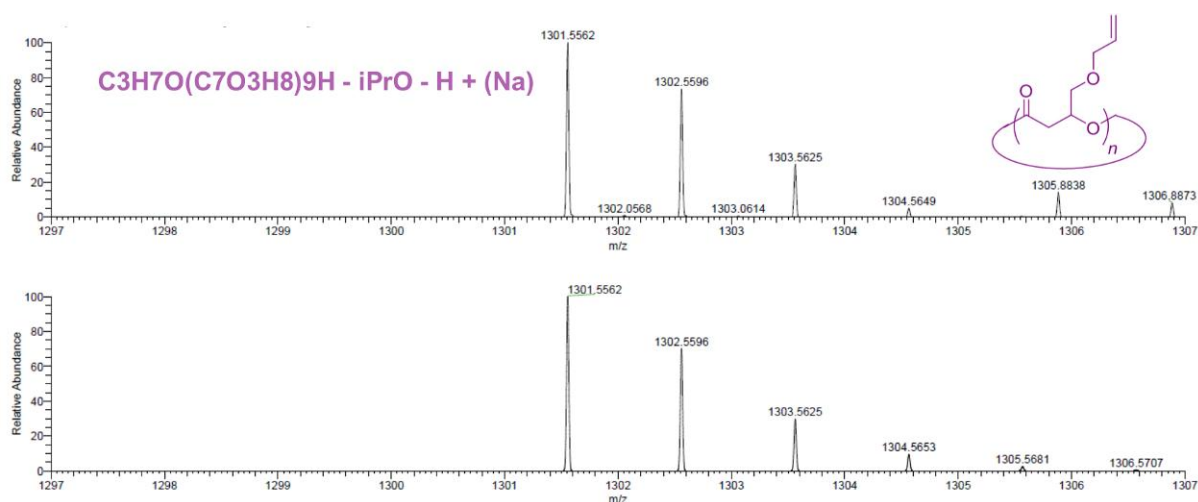


Figure S14. Top: ESI mass spectrum of a *syndiotactic* PHB^{OAlI} prepared from the ROP of *rac*-BPL^{OAlI} with the **1g**/*i*PrOH (1:1) system ($P_r = 0.88$; Table 1, entry 6) with end-chain fragmentation. Bottom: Simulation cyclic PHB^{OAlI} for $n = 9$.

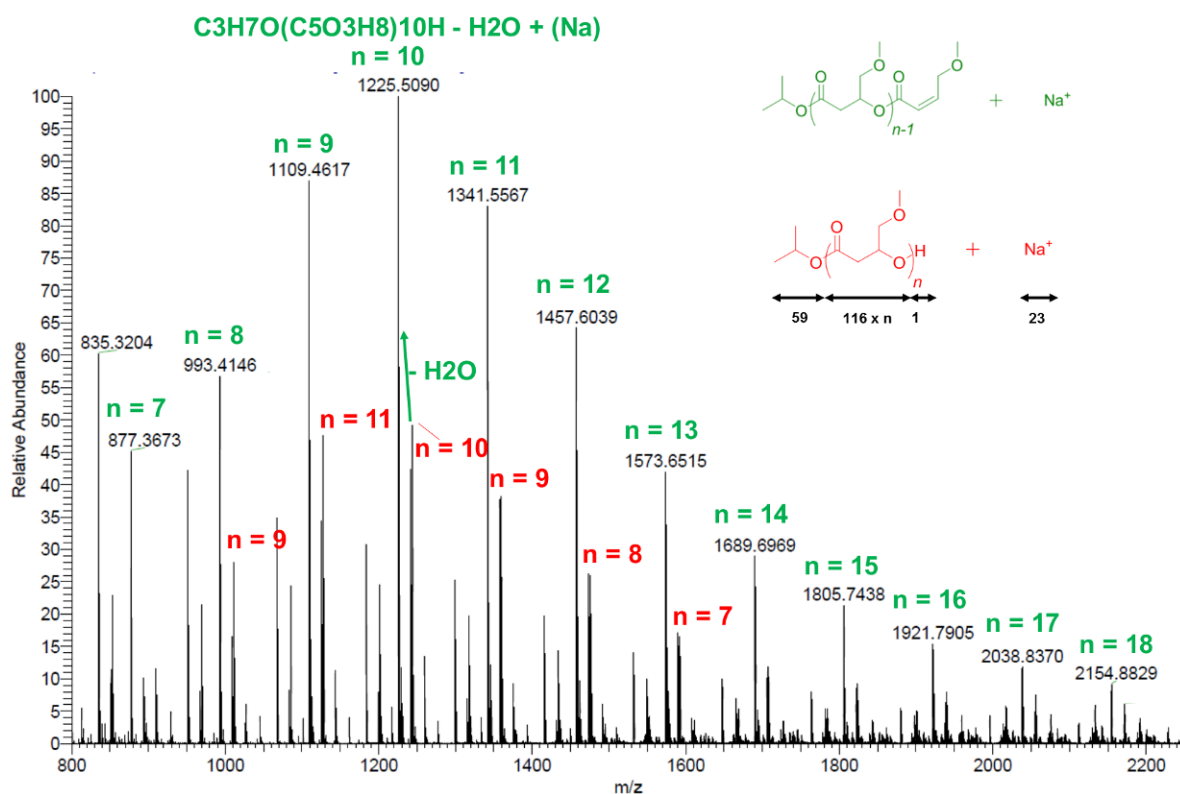


Figure S15. ESI mass spectrum of a *syndiotactic* PHB^{OMe} prepared from the ROP of *rac*-BPL^{OMe} with the **1g**/*i*PrOH (1:1) system ($P_r = 0.81$; Table 1, entry 10). The major population corresponds to H₂O-depleted macromolecules ionized by Na⁺ and the second to the expected *i*PrO-PHB^{OMe}-H.

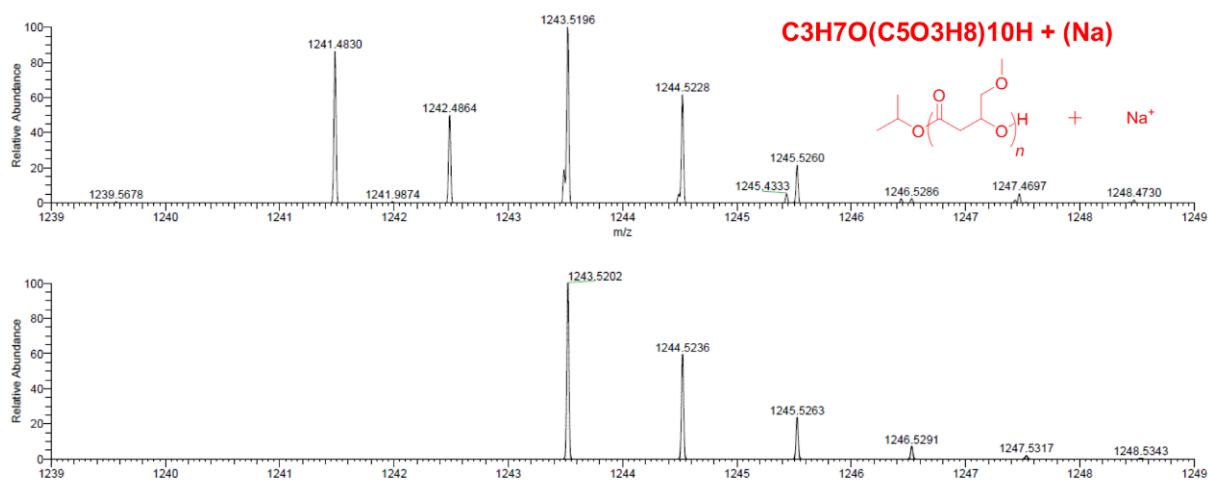


Figure S16. Top: ESI mass spectrum of a *syndiotactic* PHB^{OMe} prepared from the ROP of *rac*-BPL^{OMe} with the **1g**/*i*PrOH (1:1) system ($P_r = 0.81$; Table 1, entry 10). Bottom: Simulation of *i*PrO-PHB^{OMe}-H for $n = 10$.

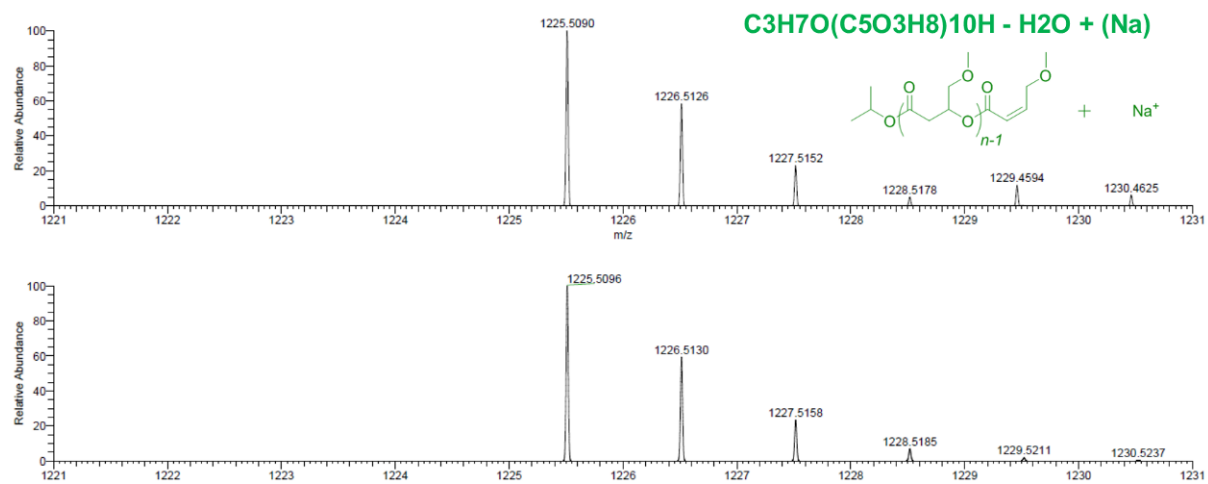


Figure S17. Top: ESI mass spectrum of a *syndiotactic* PHB^{OMe} prepared from the ROP of *rac*-BPL^{OMe} with the **1g**/*i*PrOH (1:1) system ($P_r = 0.81$; Table 1, entry 10) with H₂O fragmentation. Bottom: Simulation of *i*PrO-PHB^{OMe}-CO(CH₂)₂CH₂OAll for $n = 10$.

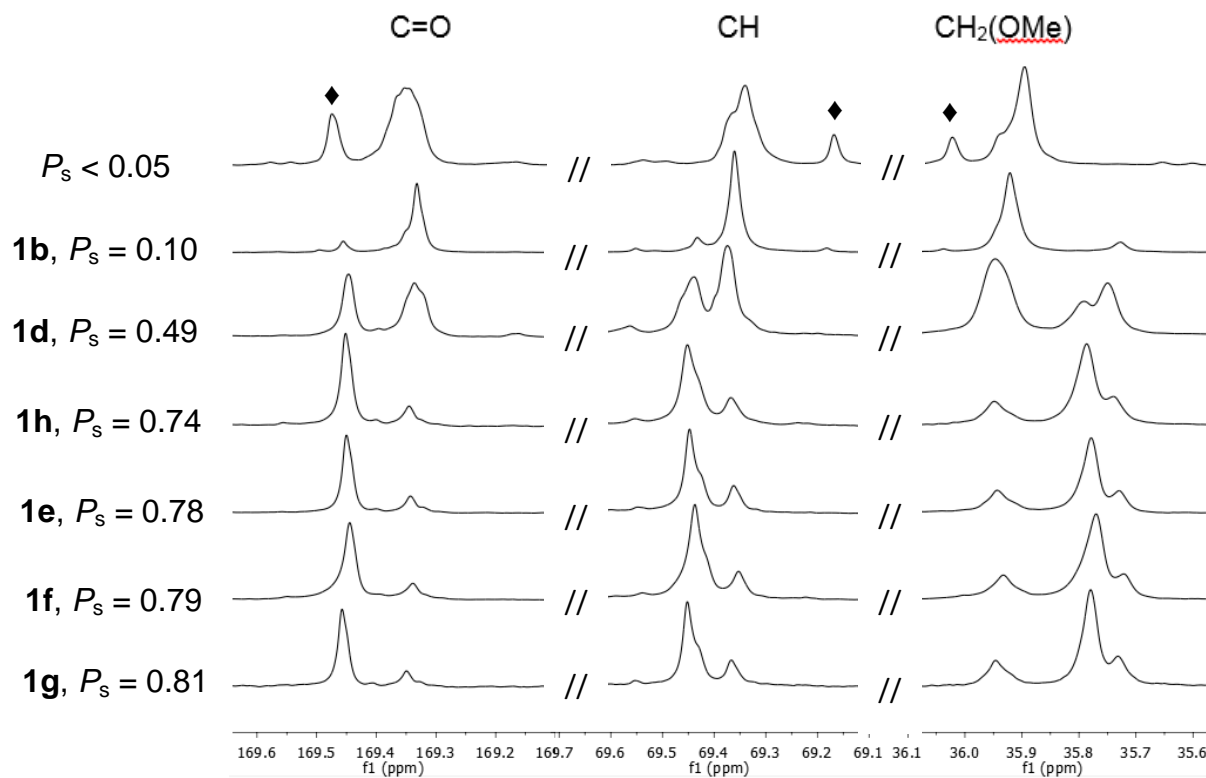


Figure S18. Detailed regions of $^{13}\text{C}\{^1\text{H}\}$ NMR spectra (125 MHz, CDCl_3 , 23 °C) of PHB^{OMe} prepared from the ROP of *rac*-BPL^{OMe} (except top spectrum, from *enantiopure* (*R*)-BPL^{OMe}) by **1**/*i*PrOH (1:1) systems (Tables 1 and S1).

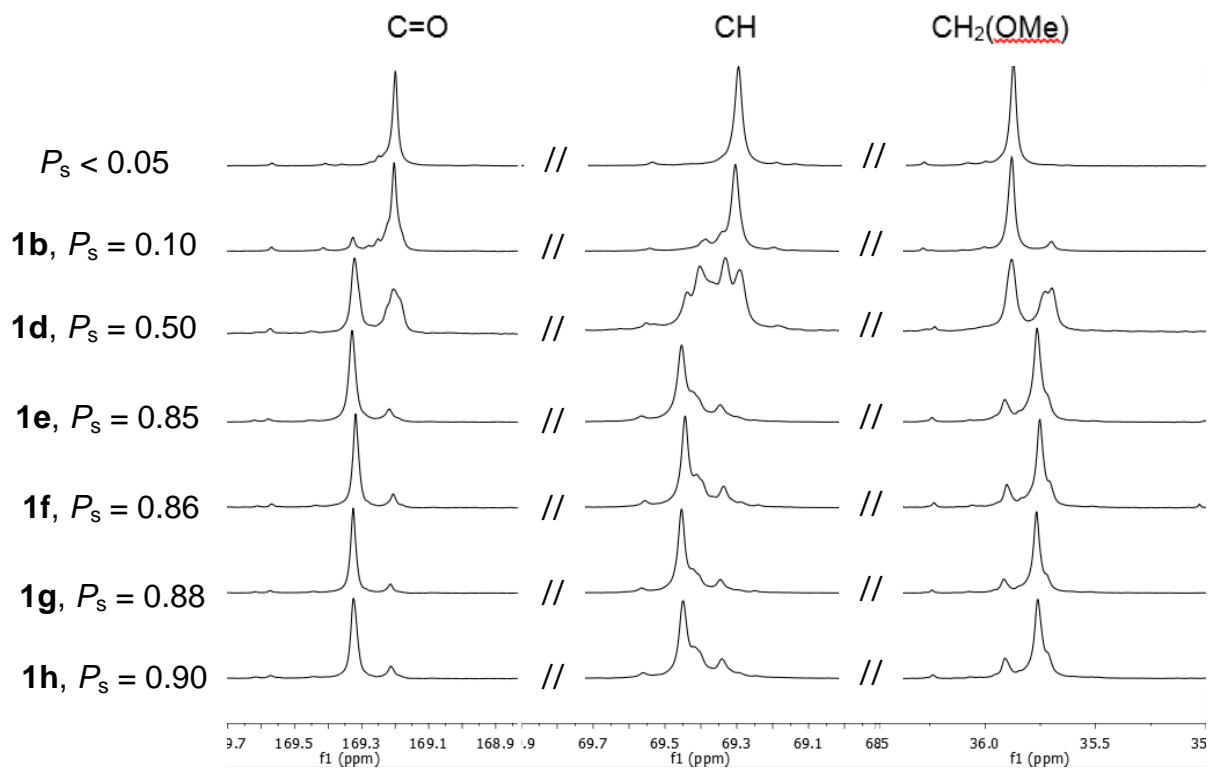


Figure S19. Details of $^{13}\text{C}\{^1\text{H}\}$ NMR spectra (125 MHz, CDCl_3 , 23 °C) of PHB^{OBn} prepared from the ROP of *rac*-BPL^{OBn} by **1**/*i*PrOH (1:1) systems (Tables 1 and S1).

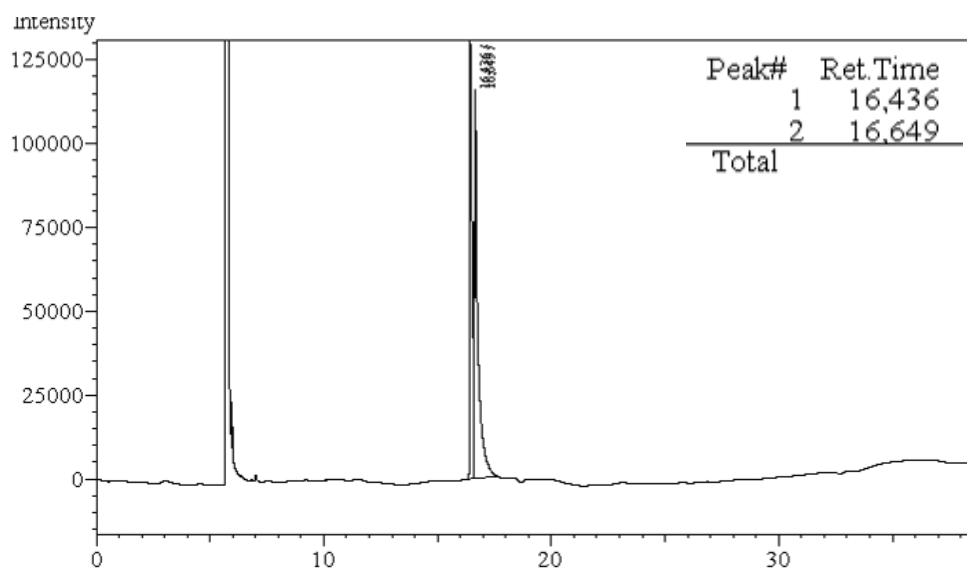


Figure S20. Chiral GLC analysis of *rac*-BPL^{OAll} prepared from the carbonylation of *rac*-glycidyl allyl ether.

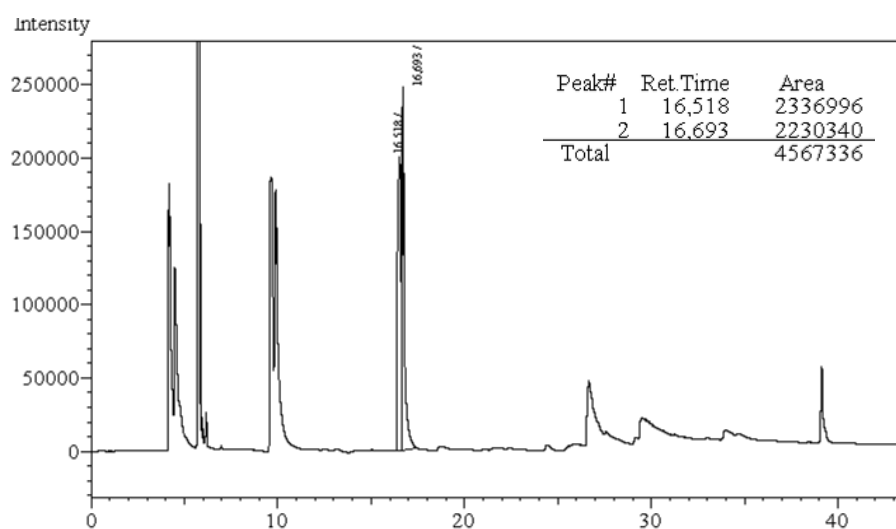


Figure S21. Chiral GLC analysis of the crude *rac*-BPL^{OAll} from the ROP BPL^{OAll} with the **1a**/*i*PrOH system (17% monomer conversion after 2 h).

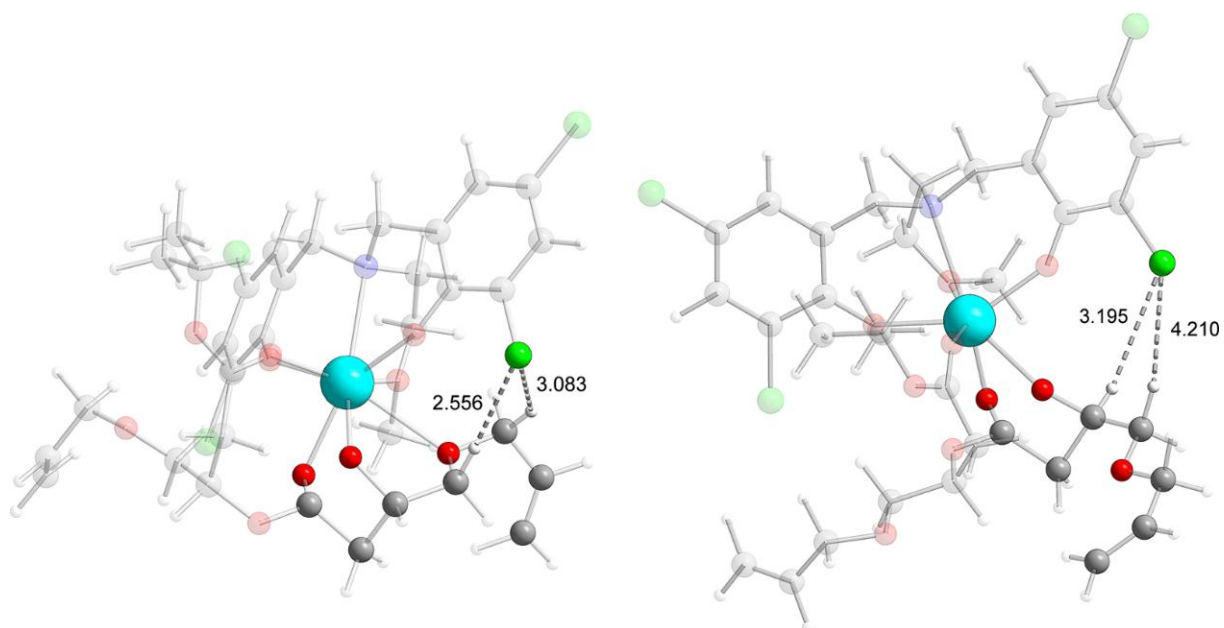


Figure S22. Shortest CH...Cl distances in **III-SS-TS** (left) and **III-SR-TS** (right).

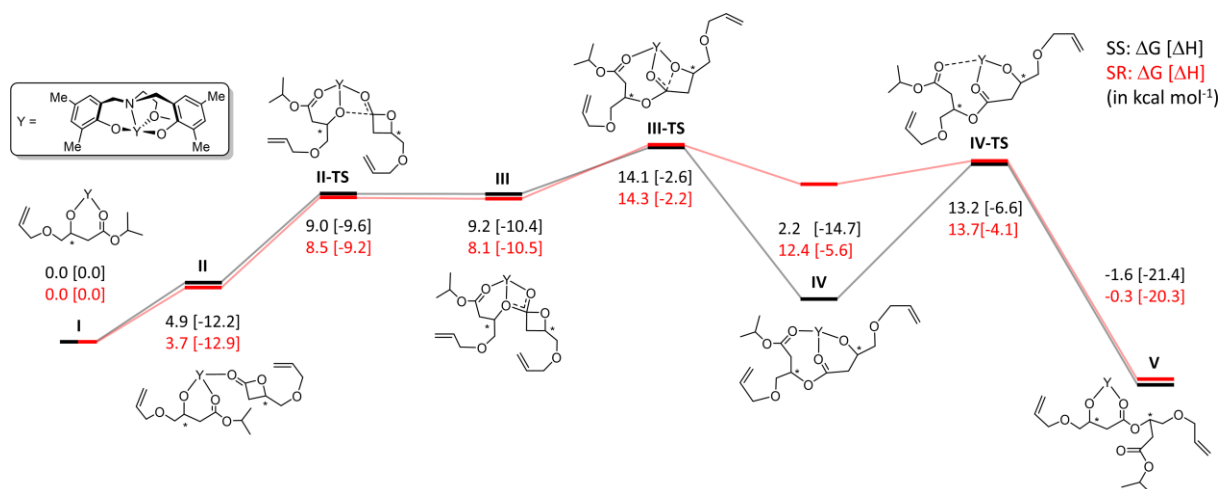


Figure S23. Proposed ROP mechanism and energetics for *isotactic* (black) and *syndiotactic* (red) polymer formation with **1c** as initiator.

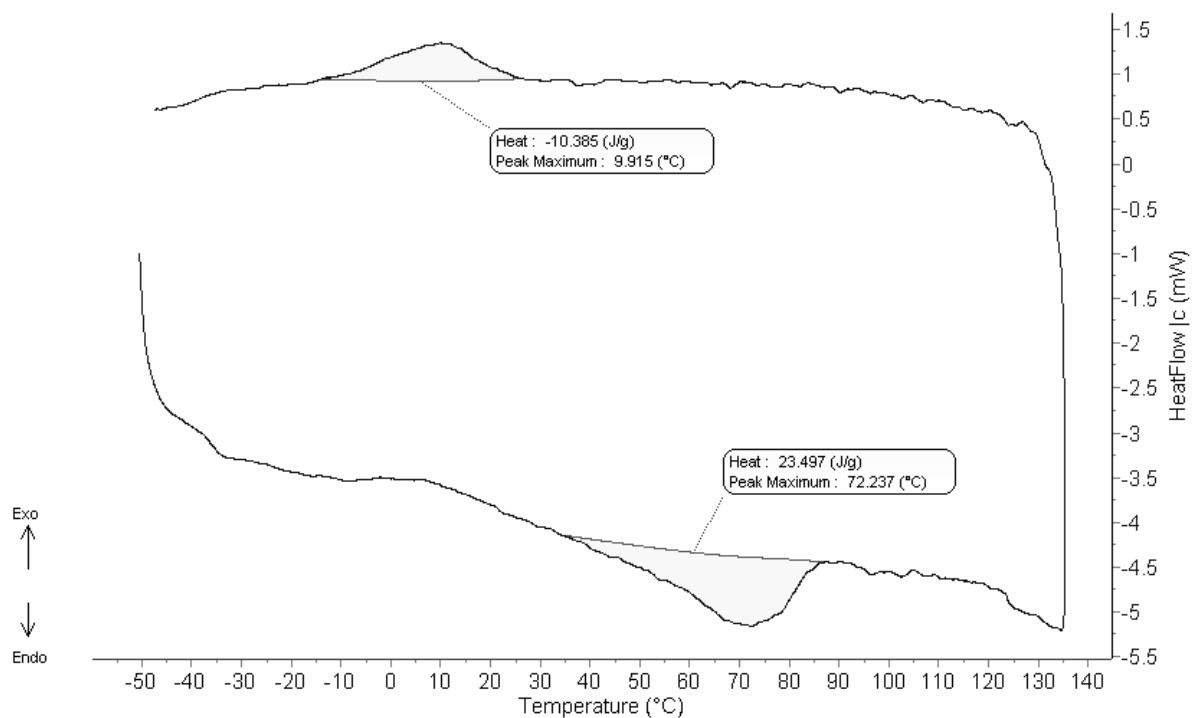


Figure S24. DSC thermogram (second heating cycle; heating rate = $10\text{ }^{\circ}\text{C}\cdot\text{min}^{-1}$; from -80 to $140\text{ }^{\circ}\text{C}$; helium flow) of a *syndiotactic* PHB^{OAll} sample prepared from the ROP of *rac*-BPL^{OAll} with the **1e**/*i*PrOH (1:1) system ($P_r = 0.81$; Table S1, entry 4; Table S3) ($\Delta H_{\text{melt}} = 23.5\text{ J}\cdot\text{g}^{-1}$).

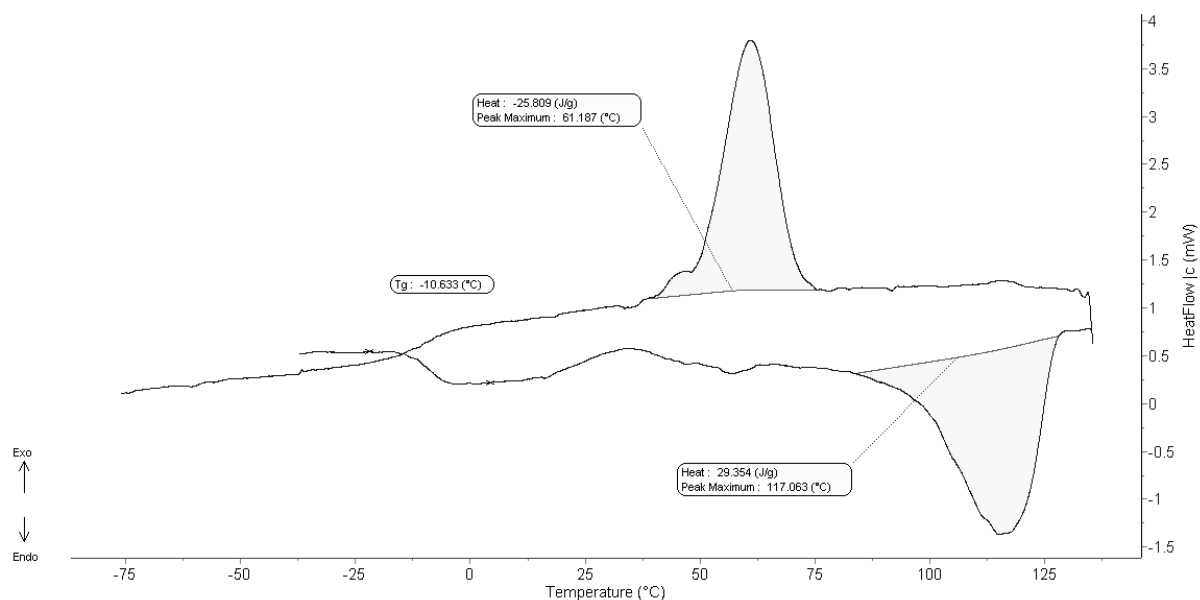


Figure S25. DSC thermogram (second heating cycle; heating rate = $10\text{ }^{\circ}\text{C}\cdot\text{min}^{-1}$; from -80 to $40\text{ }^{\circ}\text{C}$; helium flow) of a *syndiotactic* PHB^{OMe} prepared from the ROP of *rac*-BPL^{OMe} with the **1g**/*i*PrOH system ($P_r = 0.81$; Table 1, entry 10; Table S3) ($\Delta H_{\text{melt}} = 29.5\text{ J}\cdot\text{g}^{-1}$).

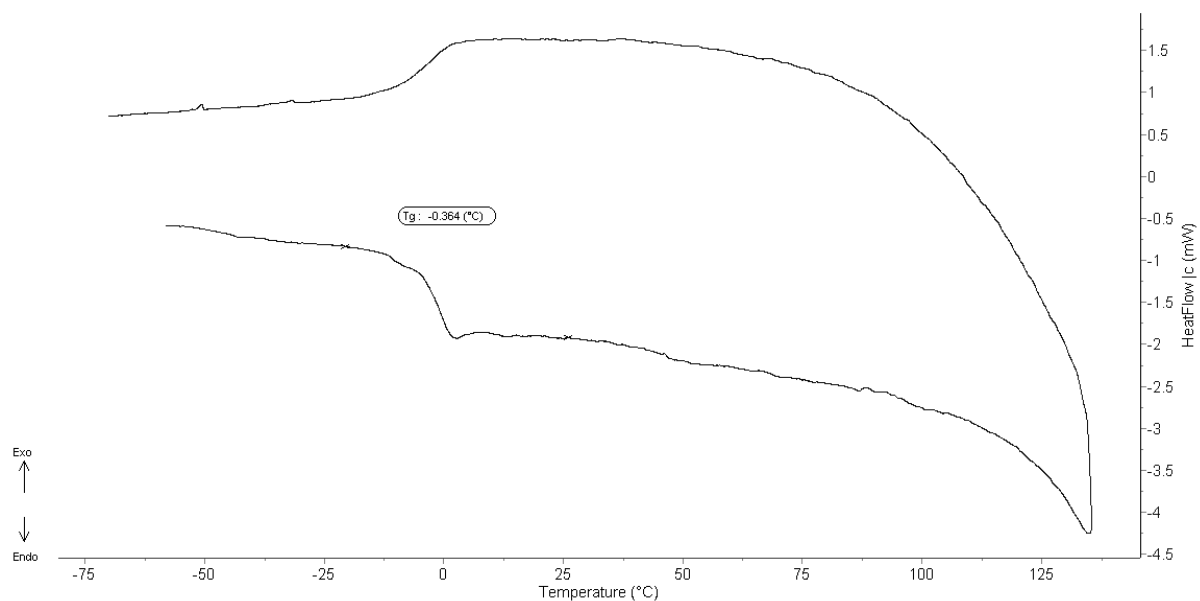


Figure S26. DSC thermogram (second heating cycle; heating rate = $10\text{ }^{\circ}\text{C}\cdot\text{min}^{-1}$; from -80 to $140\text{ }^{\circ}\text{C}$; helium flow) of a *syndiotactic* PHB^{OBn} sample prepared from the ROP of *rac*- BPL^{OBn} with the **1h**/*i*PrOH system ($P_r = 0.90$; Table 1, entry 14; Table S3).

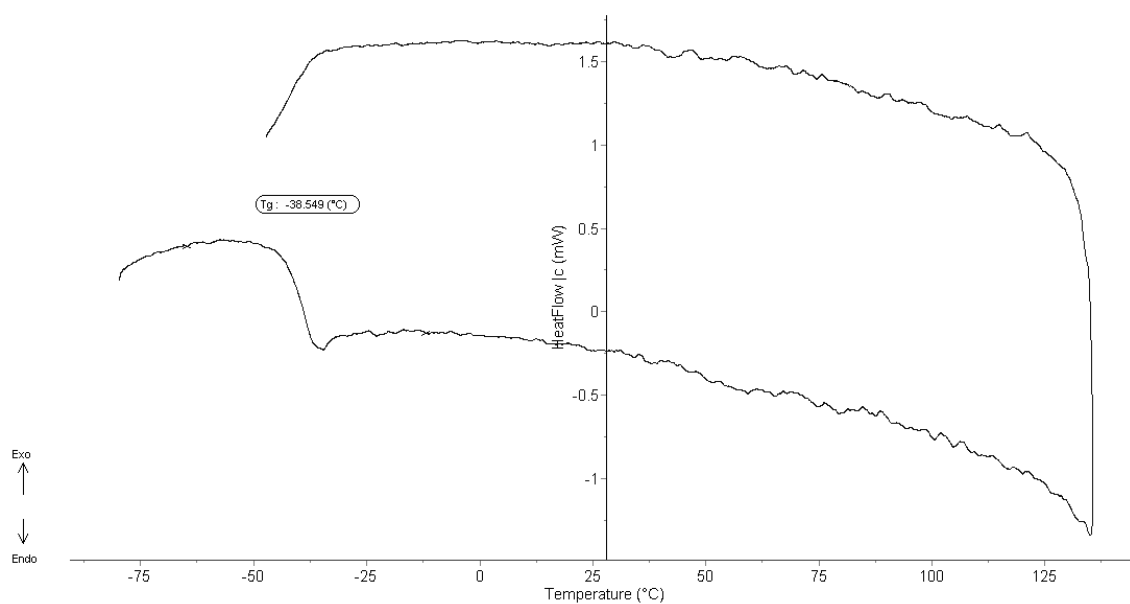


Figure S27. DSC thermogram (second heating cycle; heating rate = $10\text{ }^{\circ}\text{C}\cdot\text{min}^{-1}$; from -80 to $140\text{ }^{\circ}\text{C}$; helium flow) of an *isotactic* PHB^{OAll} sample prepared from the ROP of (*S*)- BPL^{OAll} with the **1g**/*i*PrOH (1:1) system ($P_r < 0.05$; Table S1, entry 7; Table S3).

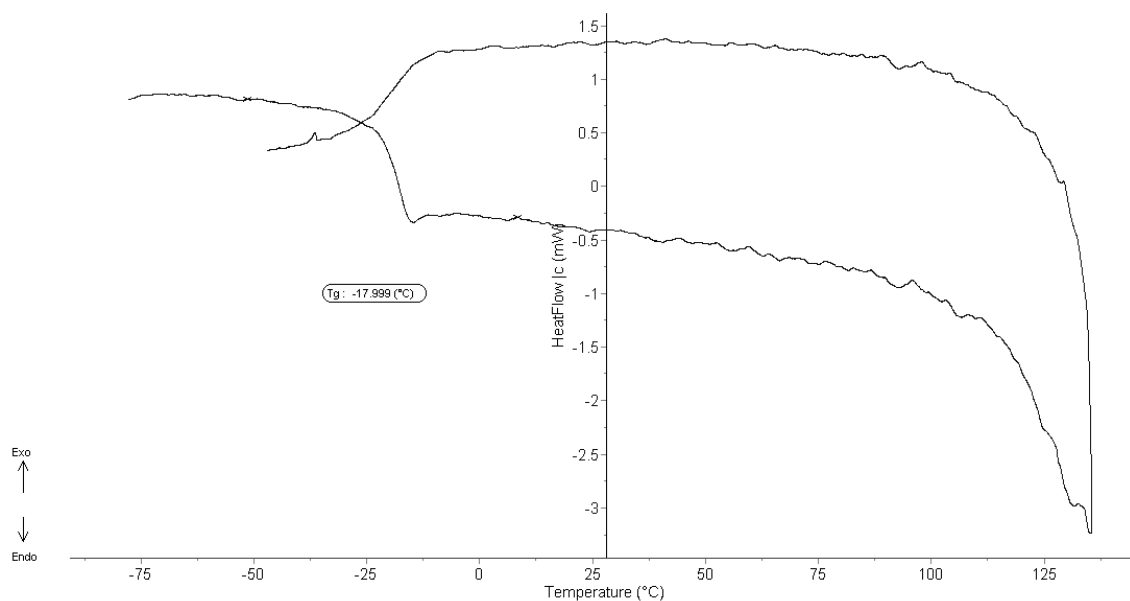


Figure S28. DSC thermogram (second heating cycle; heating rate = $10\text{ }^{\circ}\text{C}\cdot\text{min}^{-1}$; from -80 to $140\text{ }^{\circ}\text{C}$; helium flow) of an *isotactic* PHB^{OMe} sample prepared from the ROP of (*R*)-BPL^{OMe} with the **1g**/*i*PrOH (1:1) system ($P_r < 0.05$; Table S1, entry 10; Table S3).

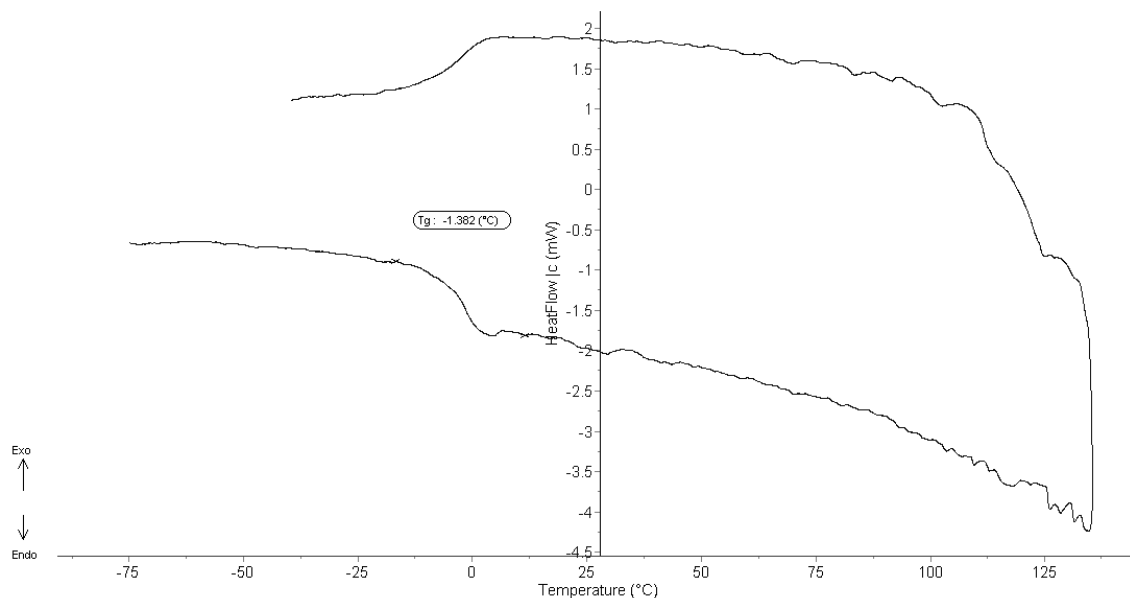


Figure S29. DSC thermogram (second heating cycle; heating rate = $10\text{ }^{\circ}\text{C}\cdot\text{min}^{-1}$; from -80 to $140\text{ }^{\circ}\text{C}$; helium flow) of an *isotactic* PHB^{OBn} sample prepared from the ROP of (*R*)-BPL^{OBn} with the **1g**/*i*PrOH (1:1) system ($P_r < 0.05$; Table S1, entry 15; Table S3).

XYZ coordinates of the optimized geometries

XYZ coordinates of the optimized geometries

{ONOO^{Cl2}}

I-S

72

Coordinates from ORCA-job 1-S

C	5.17601128800576	-3.94821279097836	-1.08235678280092
C	4.13305640135286	-3.40566222950154	-0.31115382050830
C	4.33182931516801	-2.22034786727380	0.46768501021544
C	5.63104883792154	-1.62866130783374	0.40874161305947
C	6.66904006413016	-2.16230357123773	-0.36512567156345
C	6.43360880192518	-3.32693005889000	-1.11359507853412
C	2.80767474251737	-4.11878301442748	-0.19839422924056
N	1.57943350329240	-3.40556417458678	-0.66519650304520
C	1.57407149533113	-3.13790862811659	-2.11603446746933
C	2.43566426229571	-1.95642555381656	-2.53825966206508
O	2.12797171330215	-0.81834435423405	-1.71908388178430
C	2.79685683986876	0.37757782919723	-2.16532802961892
O	3.36048280908043	-1.70607873477390	1.18760924150843
Y	1.37846393177708	-1.02766647771558	0.59504894550713
O	1.17514402759631	1.06537245136937	0.42728914740518
C	1.14853585810946	2.18740966936518	1.22187634023551
C	1.72667974312325	3.42576722746083	0.48366923130572
O	2.89897577849383	3.20564215423972	-0.27193652466390
C	4.12402769002254	3.14008002449536	0.42837048295317
C	5.28013819387477	3.42180369849901	-0.48851608451353
C	5.17273111434454	3.81593596062241	-1.76807153749802
Cl	5.92513567192672	-0.18705837509879	1.35518624002329
Cl	7.72168770781196	-4.00863048954146	-2.08383620770184
C	0.41737475652033	-4.27839662617779	-0.29520179353718
C	-0.95437551982263	-3.75259547795938	-0.63168096097248
C	-1.39411637031449	-2.56149119366621	0.02627233714070
C	-2.73096069866484	-2.13398807642687	-0.23652422457463
C	-3.58484368011678	-2.83617418591232	-1.09575826577502
C	-3.11603842220649	-3.99996249129728	-1.72712394131462
C	-1.81046606798247	-4.45744852107378	-1.49695997477798
Cl	-3.30039039828700	-0.68037871643452	0.54595864573497
O	-0.59195774028122	-1.89561788407469	0.82835249629033
Cl	-4.17326880610069	-4.88370176647537	-2.80764971267724
O	1.13058162897954	-0.37371186696264	2.84989181337613
C	1.14286178704847	0.78531428713134	3.30124225280173
C	1.84132765397795	1.92115357320144	2.60900034185175
O	0.49077033545679	1.13870881679302	4.40015396256180
C	-0.38730267011225	0.18292126966861	5.11642190469495
C	-1.58229910027157	-0.21091608566491	4.25448632720310

C	0.40283235478230	-0.98204757261283	5.70284862913997
H	2.62767160510760	-4.34505381370885	0.87555531851563
H	2.87645010193505	-5.10023312193490	-0.72800134306674
H	0.48823024257605	-4.42566334150096	0.80461499678213
H	0.55083587779635	-5.28269236455871	-0.76539323046556
H	0.52123396680650	-2.93317901796740	-2.40131319843712
H	1.89630375684552	-4.03525768388095	-2.70191754928097
H	2.20903440102655	-1.71184401280357	-3.60133065341856
H	3.52192909956887	-2.17573919903145	-2.46159692229662
H	2.45501313323611	0.63645802851046	-3.19066727588828
H	3.89699351624847	0.21912866033101	-2.17241870888310
H	2.53477059150930	1.18535339978119	-1.45619786310317
H	7.65196153714995	-1.67296352037464	-0.38257975320517
H	5.01221584373213	-4.86813079816071	-1.66388504054457
H	-1.46326181595023	-5.37748140896228	-1.99087406215883
H	-4.60567593458933	-2.47325782766195	-1.27494039115514
H	-0.73945176117038	0.82706900274114	5.94754222993964
H	2.89243094406409	1.61560217753539	2.43225584502912
H	1.81821214202323	2.82383500934858	3.24832022323055
H	0.09354700482876	2.48968923309841	1.47206147833499
H	4.28475091757474	2.13402757851222	0.88886446378846
H	4.13282935348855	3.87508920690809	1.27550312619526
H	6.27413756847081	3.26412658458957	-0.03300605037270
H	4.18270328181574	3.96848043071485	-2.22476465271631
H	6.06473036235687	3.99727314869400	-2.38681597060895
H	-0.24472434733734	-1.53021539143661	6.41633933137986
H	1.28736298520146	-0.61749251528019	6.26190589120131
H	0.73815642877991	-1.68717034290866	4.92024760271140
H	-1.29888051819822	-0.84653911590903	3.39376735068215
H	-2.10274611658461	0.68834755548823	3.86980626878557
H	-2.30490222168611	-0.77366745718253	4.87918112123371
H	0.96465313134720	3.73734886545568	-0.26022162446555
H	1.86466208814958	4.27095918227601	1.20418643388540

II-SS

92

Coordinates from ORCA-job 2-SS

C	3.04059305872184	-5.29778985168240	-1.41581851358669
C	2.14886894985724	-4.23923059038972	-1.17153448838213
C	2.48225759106869	-3.19119248037317	-0.25055194663499
C	3.74428402091888	-3.30966530995584	0.41147815413706
C	4.63065600031293	-4.36780738121459	0.17342779058851
C	4.27417056122510	-5.36103197748822	-0.75083859647748
C	0.77921816662906	-4.24921133650999	-1.80679870581022
N	0.40011753152329	-3.09119794674388	-2.66816415311611
C	1.38403922257416	-2.81415836223583	-3.73462054247951
C	2.41909398246709	-1.77716016815476	-3.30531155393845
O	1.77535706168125	-0.59596474511958	-2.80538062920383

C	1.54085421795386	0.43745020708352	-3.76826062068923
O	1.68100395258176	-2.17582932763183	-0.05210105973143
Y	0.15088644673583	-0.90963350987655	-0.96343677196267
O	0.47269440604870	1.19011735088915	-0.94475635124160
C	0.50715958655402	2.29294101497206	-0.13163665960466
C	1.92005152275182	2.60641433846538	0.38009872329310
O	2.34535997359628	1.57445143785648	1.25052220796331
C	3.67598790506937	1.72739319134699	1.72855370467372
C	4.72444221993716	1.52674860382698	0.66557707636120
C	5.68397541784000	2.41799300615737	0.36317424274121
Cl	4.19819022515896	-2.07591116315232	1.56650748051641
Cl	5.37390820017181	-6.68767353365035	-1.06884750704596
C	-0.93750596456799	-3.40732005743682	-3.24448774957699
C	-1.56885879566894	-2.36018287764557	-4.12930146212163
C	-1.92415793871164	-1.09626132437349	-3.55238055369475
C	-2.71945782825939	-0.23076188021891	-4.36684805163274
C	-3.08043898578300	-0.54332605038684	-5.68270162606295
C	-2.66244847756113	-1.76667535458119	-6.22811252682618
C	-1.92309636204497	-2.67215421449232	-5.45378514317276
Cl	-3.29004383892993	1.26729766828995	-3.65585995498254
O	-1.55877260306735	-0.76347998145838	-2.34255180057942
Cl	-3.11612444229672	-2.18508649590753	-7.86951750969183
O	-0.43847111282395	-0.23065314495275	1.27523259764754
C	-0.37359115587439	0.88553378259215	1.81844243621237
C	-0.50957901807231	2.17580573175806	1.05968113577642
O	-0.23977340966092	1.04099125368667	3.13117402613063
C	-0.05475402732647	-0.11854692086089	4.02782186863751
C	-1.27572151635897	-1.03531516653698	4.03497057127392
C	1.26979863744175	-0.82252499878128	3.76000841379564
H	0.00893922343637	-4.29782549377789	-1.00593379206198
H	0.68041774167273	-5.18980240442569	-2.40343903600688
H	-1.60806342968885	-3.59443365070522	-2.37865049675805
H	-0.87810489848690	-4.36803350274770	-3.81424109495419
H	0.82744727845012	-2.41921012481457	-4.60913379978242
H	1.90429408171732	-3.74250508417481	-4.07340089024756
H	3.08049298154055	-1.51349774624805	-4.15946127934112
H	3.05848347632253	-2.15725661329589	-2.48642949216874
H	0.86017799664959	0.09669178783948	-4.57924040105609
H	2.50521485291199	0.77353836456916	-4.20785547388306
H	1.07102012912960	1.26528657321180	-3.20501306383223
H	5.59140542703967	-4.41087264644976	0.70348390998419
H	2.76753405984542	-6.09418720989489	-2.12456013558248
H	-1.64416926100642	-3.64743174520630	-5.88094275939849
H	-3.68362589600167	0.15944696146675	-6.27296781289019
H	0.00179535167716	0.39715650379604	5.00831471012878
H	-0.43185182476160	3.03491894297336	1.75246154826925
H	-1.52455582639841	2.17844901623565	0.60831742944619
H	0.18741250803073	3.21858223355278	-0.68341519687800
H	3.79317544636599	0.94671259350335	2.51099061417107

H	3.80870111762209	2.72470913898902	2.21842072999486
H	4.67523195108589	0.55571305635223	0.14094489182753
H	5.74905490448039	3.39075532789192	0.88124587023158
H	6.44836771782851	2.20965950165877	-0.40219609498603
H	2.10557163862653	-0.09734709885407	3.78383857988209
H	1.28423311823742	-1.33738449554978	2.78096601002578
H	1.44747539821294	-1.57396498057583	4.55557261201913
H	-1.33992074630918	-1.63730969530263	3.10962618654437
H	-2.20869262716744	-0.44893026277710	4.15919407808274
H	-1.19912977491028	-1.72875446190968	4.89652210265090
H	2.59640681926452	2.69439645468897	-0.50184571248632
H	1.92868174371039	3.59348769469970	0.91155129968076
O	-1.61900107067831	-2.48001652502777	-0.00976804786428
C	-2.77647456302951	-2.14104052582680	0.15804201298020
O	-3.81278602445828	-2.95486826809853	0.47699929369086
C	-3.58188793285098	-0.86319777485645	0.11590930717928
C	-4.75600159768882	-1.79937539612858	0.45650200671560
H	-3.29424014682834	-0.12609852774523	0.88889590431583
H	-3.58423264236310	-0.39640758133714	-0.88899842086781
C	-5.84595978412106	-1.96589116523070	-0.58108289885708
H	-5.19334647104758	-1.67566386795132	1.46795433079041
O	-5.26440338933703	-2.19211726328228	-1.83710790561632
H	-6.52571322814682	-2.80410419103971	-0.28600344453928
H	-6.45462563597380	-1.02712053038033	-0.55432068193004
C	-6.07874241676745	-1.86110980527883	-2.95246911357807
C	-5.75199854466830	-2.71867887908206	-4.13961775722702
H	-7.16159142566665	-1.98918281600710	-2.69937135190657
H	-5.94308708265001	-0.78149235210822	-3.21423783259319
C	-4.95774179758778	-3.80045246172655	-4.11398550623878
H	-6.22054165710367	-2.39378563310660	-5.08544330062092
H	-4.75759717278832	-4.37704442237544	-5.02918647160170
H	-4.47352147718455	-4.12200038324222	-3.17926011435831

II-SR

92

Coordinates from ORCA-job 2-SR

C	4.76000978931555	-1.78413131940369	-3.85280063957436
C	3.97649930590154	-2.37799755621557	-2.84865563076447
C	4.57990685068247	-2.91478493498960	-1.66331559330029
C	6.00494292320668	-2.82731077477267	-1.58184162460995
C	6.78681982084701	-2.23953645140333	-2.58404531189290
C	6.15504534655996	-1.71285974278414	-3.72105305490850
C	2.48745271334607	-2.53664534448968	-3.04421390517632
N	1.58474332645802	-1.88413821208719	-2.05208332537758
C	1.85098682969225	-0.44065041026742	-1.88414199764320
C	2.85363302182272	-0.16388591905940	-0.76557916757336
O	2.45572595276269	-0.82274394019677	0.44427742727642
C	1.75107941814969	-0.01779876163959	1.39461383520750

O	3.85511095476161	-3.43222023140676	-0.70509976066645
Y	1.94486929790002	-3.24804849572575	0.34011201993379
O	0.94947872893165	-5.10799312666544	-1.11793180103644
C	-0.09669237876509	-5.70375862458380	-0.94629267010345
O	-0.24909025828469	-7.05114148392242	-0.91601359932538
C	-1.70983570242534	-6.90817732248004	-0.65384867198251
C	-2.10163978716929	-7.52125374169509	0.67404529173897
Cl	6.79764549235285	-3.48422126486296	-0.16496553985658
Cl	7.11659123036928	-0.96877040645700	-4.98243095969561
C	0.18769732206975	-2.12616973558157	-2.51116721168856
C	-0.91820411720321	-1.53817891833206	-1.66517226026939
C	-1.05143470704700	-1.94085710088028	-0.29438205560629
C	-2.19201166026177	-1.43556108271253	0.40891290976052
C	-3.12649929570588	-0.57452785457446	-0.17793153911297
C	-2.94740522253648	-0.18594332188278	-1.51507180444440
C	-1.85493833280843	-0.66625365533170	-2.25137428636257
Cl	-2.41710213229477	-1.94121736705493	2.06781858199919
O	-0.18864334479316	-2.73475172316854	0.28575839071105
Cl	-4.10086289341668	0.89802368409873	-2.26597686464785
O	2.45430993642209	-5.43666343603455	1.18633298027997
C	2.93156961893572	-5.78627517276023	2.27920752724497
C	2.70059149935806	-5.05487814385461	3.56665439148561
C	2.98682908958844	-3.52404239977556	3.44036319875757
C	4.48934679870784	-3.24599349405795	3.26495407779241
O	5.22553926539478	-3.83005339713485	4.32843129083461
C	6.63419814817138	-3.71946201224384	4.17366431429723
C	7.14769651400339	-2.31395653958054	4.35904574604012
C	7.82115899492287	-1.61630104852394	3.42805925559900
O	2.28035723853674	-2.94049251362286	2.40829755729158
O	3.70334452226094	-6.86599967788322	2.38902936766824
C	3.99923090855804	-7.64150873989386	1.17189199295360
C	5.18858558347811	-7.01508160929250	0.45535373330490
C	4.23264779972391	-9.06944497831299	1.64115096626377
C	-1.55906985069004	-5.37595311762056	-0.72404833110583
O	-1.56358448370795	-6.76039445357066	1.72432580793523
C	-1.78951639436776	-7.31474279761347	3.00504418475858
C	-1.43190714688175	-6.35013723724399	4.09670577455771
C	-1.08003663357143	-5.06437062935295	3.92651572320400
H	2.23460587025791	-3.61992691353419	-3.02137890655917
H	2.22910168904370	-2.16723534528383	-4.06781168355254
H	0.07395938680159	-3.23004154075072	-2.55916794211660
H	0.06790204883413	-1.75080211552503	-3.55804082947878
H	0.88901432100548	0.04814202268924	-1.62741536112890
H	2.21087012337590	0.02916111768705	-2.83173219686107
H	2.93940668236890	0.93058432756106	-0.59078394253121
H	3.86123944014315	-0.54408750465434	-1.01996215124889
H	0.77822062174201	0.33856244763539	0.98956885322609
H	2.37309007601507	0.85443814310198	1.69201073037798
H	1.58036121576948	-0.67090941703056	2.27100065970082

H	7.87837592481803	-2.19120449719190	-2.47429968471702
H	4.28130845157143	-1.37904827693766	-4.75716763961064
H	-1.73836029463138	-0.36334237806680	-3.30305288298905
H	-3.98295309848113	-0.20955092486706	0.40453935279830
H	3.09959449310072	-7.57901107973288	0.52502171586649
H	3.31386780960298	-5.50038248153912	4.37125812116056
H	1.62412881910345	-5.17309157269517	3.81674622377794
H	2.68883308262848	-3.09615806271156	4.43254638917346
H	6.95603761667664	-4.11118526249438	3.17675738578687
H	7.06795627681287	-4.38305801670984	4.95360468406458
H	6.92451782469426	-1.85399345381077	5.33965586766906
H	8.03157036196983	-2.04360469741772	2.43238762200486
H	8.18160293378046	-0.59287769438759	3.61950887809923
H	-2.04355974406470	-4.86312299817943	-1.57689544148596
H	-1.74892007256521	-4.81431473875028	0.20947817594178
H	-2.26955515155427	-7.38266322237530	-1.48439274810401
H	-1.20663778715010	-8.26438686397483	3.12932452493033
H	-2.86658014463667	-7.60841855727031	3.11781992300969
H	-1.49335648594324	-6.77951815364186	5.11291148409627
H	-0.84984890866002	-4.42576527017185	4.79307209317781
H	-1.01686648576553	-4.59887978983373	2.93107789976089
H	4.97037705066862	-5.97703175630195	0.13796689011710
H	5.42991456707965	-7.60438066807629	-0.45229374857445
H	6.08381452691282	-7.00901417041118	1.11007986551878
H	3.34737443020579	-9.46363497656148	2.17794503244732
H	5.10664656271235	-9.12504949562185	2.32124323690173
H	4.43006594938779	-9.72449652780114	0.76961704952786
H	4.83148731888893	-3.64724745175485	2.27689995006212
H	4.63229937894790	-2.14045515291662	3.22112652485183
H	-1.73857456628964	-8.57944636497860	0.69911149681833
H	-3.22037101643994	-7.56142412581064	0.72592378791882

II-SS-TS

92

Coordinates from ORCA-job 2-SS-ts

C	2.58549759693834	-1.78644622632749	-4.59911085140213
C	2.66342680111892	-2.06709684416565	-3.22364884392177
C	1.98730927732299	-1.24065071819313	-2.26812493729746
C	1.27882540134586	-0.11066597952186	-2.78303872872895
C	1.20732922699276	0.17235311788633	-4.15266476137685
C	1.85885819387256	-0.67814049169080	-5.06006027778845
C	3.56444955063690	-3.17426312828165	-2.72733757642988
N	2.97244619558514	-4.24467359127039	-1.87622523549351
C	1.82917163428505	-4.92523003105217	-2.52306855368585
C	0.49037740839883	-4.28962191634719	-2.15016053754693
O	0.32880527922977	-4.23116716550221	-0.72278880857758
C	-0.34285068367992	-5.35213897687461	-0.13243373424372
O	2.00999187054549	-1.51954264103708	-0.99002847095562

Y	2.16061054197933	-3.11872530556002	0.47805345698327
O	0.42158001546640	-3.10635722683159	1.97929309991701
C	0.67645936958432	-2.28058926666117	2.90215438569746
O	1.00871071729601	-2.68850332858542	4.19541876087124
C	0.26270580155703	-1.57094216682370	4.78663692347592
C	-0.84757701294612	-2.06897869049889	5.69485724447359
Cl	0.47751609344150	0.94587823441733	-1.64363883784363
Cl	1.76903157993989	-0.34552027441881	-6.77765019750621
C	4.08219997281606	-5.19733651081988	-1.55220050724335
C	3.70154183710257	-6.42967446239590	-0.77141667768523
C	3.13707807541682	-6.26704367245996	0.53422792650983
C	2.84584190495955	-7.46319925672386	1.26324279130203
C	3.10445635878509	-8.73805247913306	0.74513184404811
C	3.66205080295520	-8.85621674033301	-0.53849390732895
C	3.95622639984717	-7.71161813569003	-1.29302496913274
Cl	2.13833781464685	-7.30623741084971	2.85001355934733
O	2.88729143348489	-5.07988442080187	1.02595318400758
Cl	3.98847492220534	-10.44624858301396	-1.19866596025679
O	4.47217176750631	-2.40833228325527	0.63175896105214
C	5.08006029253173	-1.69075029348396	1.44108228794708
C	4.57859872148928	-1.35437302445754	2.82085729560696
C	3.14457401399735	-0.76026712009183	2.79747692857391
C	3.07526231712108	0.57363630057839	2.03832096240533
O	4.02033404110873	1.48394925734797	2.56696799222440
C	4.11510171179568	2.69442579212792	1.81943256804796
C	2.90146643137119	3.57659714401543	1.96411393401237
C	2.05762453479965	3.88171475472178	0.96298689870964
O	2.24460614665304	-1.65057529997108	2.21210270836642
O	6.25440566933899	-1.13328110078639	1.15509112801801
C	6.84059989693663	-1.34456661633455	-0.17679752737256
C	6.27193131111896	-0.30485413401260	-1.13590532843813
C	8.34712868119962	-1.26115575719445	0.01189731468087
C	-0.13289929966053	-1.06930608439003	3.38397923766557
O	-1.78700141586329	-2.78208483371571	4.93274039737608
C	-2.82957335523939	-3.36601666892906	5.67551222685770
C	-3.69245075779114	-4.22610659293446	4.79865252021768
C	-3.44283261344273	-4.49987211839792	3.50777347082942
H	4.37843270690136	-2.72351495648772	-2.11716506994687
H	4.05649464730046	-3.64729257663492	-3.61323014003660
H	4.82668182381036	-4.60665722068955	-0.97369990679526
H	4.58548674482673	-5.51475040948438	-2.49815243961721
H	1.83055616238577	-5.98114454859754	-2.18348086238379
H	1.93201020323091	-4.94283395194729	-3.63477155707960
H	-0.34758129782056	-4.86649839314605	-2.59867503223715
H	0.41799565057389	-3.24829276352553	-2.51701470884386
H	0.20204338458060	-6.30170170991673	-0.32389606263082
H	-1.37679939888237	-5.42607716627204	-0.53336008758632
H	-0.37949691055488	-5.16282413534029	0.95554727977950
H	0.64467443000910	1.04655483077680	-4.50640841201739

H	3.10805476160312	-2.42937444192393	-5.32355815681849
H	4.39483266688962	-7.82220293644566	-2.29631653916513
H	2.86704641846484	-9.63107957306371	1.33856151650502
H	6.54305616490297	-2.36271559499021	-0.50379294941780
H	5.27817416520563	-0.64949200082364	3.30552964422078
H	4.54131244406020	-2.29779591834936	3.40516548780081
H	2.87712778926303	-0.57972054049660	3.86740398795805
H	4.29496407749057	2.47149278295113	0.73833702773922
H	5.01482989515671	3.21242063285879	2.21514266081716
H	2.70954668286851	3.96144448271840	2.98270103302062
H	2.20701416295227	3.48828605842914	-0.05743767308431
H	1.17978261390729	4.52786739623794	1.12327777765447
H	-1.20788914001240	-1.17162589459116	3.14879487434943
H	0.24630107397857	-0.07767411408447	3.08209509536526
H	0.94154812988502	-0.90632886789436	5.36410763877056
H	-3.45943973704962	-2.57912582446504	6.17037420205522
H	-2.41897317969526	-3.98778362833212	6.51508474948327
H	-4.58255112882486	-4.64694534991782	5.29967424848177
H	-4.11883610007805	-5.14456681966518	2.92540671516763
H	-2.55250130542202	-4.09131759561153	3.00421238297858
H	5.17234830514141	-0.40045601647369	-1.22932971232431
H	6.71239089116311	-0.44010321764141	-2.14400772711312
H	6.51270791226826	0.72047517025458	-0.78895578933064
H	8.70020902134239	-2.02015222662373	0.73689026267237
H	8.64441351747523	-0.25895396654127	0.38095265850575
H	8.85832507554127	-1.44074930215378	-0.95441507759732
H	-1.31353247594584	-1.18836107851266	6.20972500424422
H	-0.39865035849793	-2.71325559234919	6.49223571240621
H	3.25707880633043	0.38335360803076	0.95021033800109
H	2.03380822717237	0.96828633945984	2.10413282708035

II-SR-TS

92

Coordinates from ORCA-job 2-SR-ts

C	5.15882158463202	-0.12414475579229	-3.02618513959430
C	4.31774680542493	-0.94263219618789	-2.25181599136821
C	4.21935267028180	-0.75929933277978	-0.83465279952145
C	5.01778133322527	0.27873092470657	-0.26225054670082
C	5.86074636897648	1.08885428371221	-1.03381981636448
C	5.92534436833735	0.88292770261807	-2.42085968932640
C	3.56985566830733	-2.08648730564523	-2.89558758205926
N	2.08313361709091	-2.10689485780835	-2.76013210190232
C	1.44549794023318	-0.85218307857134	-3.21852994714896
C	1.23097383391982	0.14271223574812	-2.07856686043644
O	0.51203257004344	-0.46820524828037	-0.99462553519397
C	-0.91039973885455	-0.31067283585660	-1.03640793128055
O	3.40982497482153	-1.49059591003475	-0.10930557126188
Y	1.52446701713203	-2.54909089123020	-0.13373565482841

O	0.24995779173096	-1.72765193368153	1.59604176060230
C	0.27723091641473	-2.51631651443230	2.57467180293574
O	-0.80483120406794	-3.31895640930592	2.92218722151128
C	-0.61662611843997	-3.00511684150508	4.34996646969437
C	-0.64160863016583	-4.20774536409623	5.26870334790639
Cl	4.91582467854749	0.54111816658331	1.46026889484461
Cl	6.97076908624721	1.89238324509138	-3.39983065778511
C	1.59086335223517	-3.28838846248270	-3.53424845111309
C	0.09379180531350	-3.47370601001378	-3.59677597429983
C	-0.63870929471124	-3.65042369021482	-2.37821317554243
C	-2.04381276763783	-3.89089165157115	-2.50244899210980
C	-2.68942255393823	-3.95994102932432	-3.74267235896542
C	-1.93718649013677	-3.78016408963663	-4.91474438581218
C	-0.55809637367657	-3.53701314947453	-4.84248267713677
Cl	-2.96957189051286	-4.10359166945950	-1.03725117026252
O	-0.05486465516728	-3.58504637703194	-1.20818021261025
Cl	-2.73052800918449	-3.86005923183533	-6.47492458516158
O	2.78204361264720	-4.55390901904083	-0.65807592673981
C	2.62282963039972	-5.67017232818733	-0.13465771703613
C	1.51070642474084	-5.98349222890704	0.82017240931021
C	1.60591048106860	-5.10604708128794	2.10563648919566
C	2.86926189528911	-5.42534991541950	2.92026635796503
O	2.85704830395638	-6.79556622762681	3.30052418810838
C	4.10000190315074	-7.26766026979359	3.80725265192678
C	4.50438995725229	-6.64344349034133	5.11796998857517
C	5.69299860056447	-6.06026738380899	5.34860959989951
O	1.57845330783020	-3.74187123949579	1.81160810030473
O	3.46100125507427	-6.68168703059026	-0.35604091892268
C	4.61622069845449	-6.46860142307076	-1.24054811995426
C	5.74674131910614	-5.82252807554497	-0.44812864598195
C	4.95772918848825	-7.83546004853967	-1.81285619663742
C	0.69593189717975	-2.26237060244921	4.02396777332766
O	0.49449523800620	-5.01947194144079	5.06897971173203
C	0.44584965554138	-6.29404313995361	5.68683121769144
C	0.89117374224295	-6.31345865373466	7.12659558468476
C	1.50250982644549	-5.29978599830551	7.76334933470851
H	3.92493283633536	-3.04514224095567	-2.45717224199032
H	3.83346536987882	-2.11010372211852	-3.98175699725867
H	2.05780803874197	-4.17740898436720	-3.05769564376914
H	1.98657313072112	-3.23850265540541	-4.57840931456673
H	0.45877878614519	-1.11692782015792	-3.65034335794300
H	2.03359476985424	-0.36146383889552	-4.03054945161140
H	0.67378968297208	1.03244821550809	-2.44494616199276
H	2.19179569868407	0.49570721494517	-1.65925283376626
H	-1.34487009170162	-0.74862904732043	-1.96106622916136
H	-1.17398270825961	0.76749219287297	-0.97391177419584
H	-1.31410171218273	-0.84141695488472	-0.15555352508284
H	6.45567322818506	1.87749496039650	-0.55420806304450
H	5.22762039003504	-0.27604339771376	-4.11399547301836

H	0.01610561984680	-3.40179099602696	-5.77158250364066
H	-3.77029426003173	-4.14786274968074	-3.79147486966713
H	4.28519190508507	-5.77976648729803	-2.04563152632081
H	1.53430687337669	-7.05320474523863	1.09638921898814
H	0.55279926153244	-5.73962839679094	0.31300806097550
H	0.72122178373008	-5.37658492238045	2.72634178806157
H	4.91186841332682	-7.12208972777661	3.05125769048565
H	3.95952116456151	-8.36309875975972	3.93876765598891
H	3.75137301270066	-6.69141580720852	5.92685391616106
H	6.46021255553436	-5.98638735184513	4.55855789830841
H	5.95075406099722	-5.64071390357060	6.33376718008686
H	0.75142329569653	-1.19193733396953	4.29548894839466
H	1.61009324849081	-2.79829734538978	4.33036612730568
H	-1.43478135750052	-2.31951585119781	4.66185182175586
H	1.11575349054807	-6.94446744607846	5.07847926389194
H	-0.58007750441612	-6.73146444304532	5.60259168769373
H	0.70518738706969	-7.26510713711922	7.65827713632739
H	1.81814663302701	-5.38809397345414	8.81397119077372
H	1.70828918569817	-4.34905745752156	7.24567611967248
H	5.44579119683027	-4.83155202408473	-0.05620892845471
H	6.62868981775818	-5.67524273180034	-1.10316609223373
H	6.05138120735513	-6.46946768678677	0.39973780250024
H	4.09405103943860	-8.26699002386387	-2.35528974773424
H	5.25169304855724	-8.53879161566226	-1.00785910336088
H	5.80410858021910	-7.74648385039000	-2.52211825165792
H	3.77992830178249	-5.19440673407316	2.31203438454621
H	2.89642520013856	-4.75707019176043	3.80964555055727
H	-1.57964226839000	-4.78184988426929	5.06696674909022
H	-0.70712290623206	-3.83861596852911	6.32205232703990

III-SS

92

Coordinates from ORCA-job 3-SS

C	4.21600952915324	-7.66121637254623	-1.13331567735109
C	3.84510773151828	-6.38645988770558	-0.66667129512537
C	3.23120220518505	-6.22471285966345	0.61485990504542
C	3.02485803626694	-7.40916571576134	1.38839263527352
C	3.40102163443044	-8.67608747899361	0.92623618228914
C	3.99685355310628	-8.79598339323473	-0.34012838273928
C	4.16125240846386	-5.15689352711091	-1.48051917895266
N	3.01233738438777	-4.25404643651361	-1.82760351690827
Y	2.19781053848043	-3.08882967892238	0.44602267515388
O	2.12759125501867	-1.40133129355747	2.12348619787045
C	2.99731396382730	-0.50227116378313	2.78996380309848
C	3.06784296140526	0.77453623008756	1.94564339705097
O	3.99003392855862	1.67089027820384	2.53233831727130
C	4.19079036842080	2.85498541788526	1.76168263992484
C	3.00035586008694	3.77906341571111	1.77931209647827

C	2.25729650540343	4.08394040878020	0.70124737498485
O	2.86397894348988	-5.04325592307362	1.04471530218488
Cl	2.27401651960104	-7.24885216146005	2.95244155001210
Cl	4.46610313442172	-10.37769558134745	-0.93067276218494
C	3.55556223839666	-3.23214843834899	-2.76921363242858
C	2.64013969733217	-2.12448428130652	-3.23122367864214
C	2.39359254322640	-1.92679689240133	-4.60089896113408
C	1.62045645456533	-0.83843418982058	-5.03359260305980
C	1.09246345328463	0.07250589271040	-4.10421528392792
C	1.34078669849468	-0.12537076230688	-2.74033760744260
C	2.11167931410153	-1.22494201887888	-2.24939638035471
O	2.31859504880745	-1.41451154377638	-0.97123871924278
Cl	0.68395635166830	1.00311020049091	-1.57488616286590
Cl	1.31778747030640	-0.60576413496308	-6.74316036748791
C	1.88383040539874	-5.02334061534805	-2.38769222066887
C	0.54148107935642	-4.30968694964867	-2.31112459601564
O	0.31822711463496	-3.84495639135584	-0.97281043191835
C	-1.00308297234087	-3.31696574871517	-0.78817570646843
O	0.47752093017695	-2.84534951201937	1.85388348946472
C	0.80872122144353	-1.90334440045090	2.69956614946188
C	-0.17385826463584	-0.78470362827199	3.13142707990482
C	0.09243669451362	-1.28812373381706	4.56194706298081
C	-1.06704464559709	-1.92582574639393	5.31099108230350
O	-1.81306444481361	-2.72146192330077	4.42811123464847
C	-2.87726606709907	-3.43042911792205	5.01214323978047
C	-3.42140682145060	-4.44889083627590	4.05128684345984
C	-2.84945561742174	-4.76570821035615	2.87765833243459
O	4.46570602773395	-2.40458979479518	0.91873556215713
C	5.00805402821790	-1.63494708268553	1.72474681818574
O	6.22521226054801	-1.13790945302779	1.52689576202671
C	6.94009386169285	-1.48335881075413	0.28719123735967
C	8.42049740528842	-1.40503534997512	0.62366882259872
O	1.04711379467672	-2.27379132058346	4.07587018205205
C	4.37367461539953	-1.16650324947652	3.01156807161756
C	6.49532740079750	-0.53104576901114	-0.81711822171559
H	4.42254175986227	-2.77542418447041	-2.24169493473999
H	3.96713074312662	-3.75443287544053	-3.66784231990680
H	4.88735311895291	-4.51955462446980	-0.92752595332754
H	4.66796094421825	-5.47794065099602	-2.42263794210651
H	1.81656716493755	-5.96627029996327	-1.80801293367287
H	2.06863750353255	-5.31173252396634	-3.45239102884434
H	-0.25903968451586	-5.03585156951197	-2.58347100672934
H	0.47576916567152	-3.45106797479206	-3.01361148279362
H	-1.75852719684514	-4.10905072091480	-0.98334272903833
H	-1.17755041682275	-2.46132655321279	-1.47734915328314
H	-1.06422095200028	-2.98155996611646	0.26299959758402
H	0.48985511050579	0.92809780558426	-4.43722184919292
H	2.81204814502045	-2.62230789314214	-5.34421657216005
H	4.68722721288935	-7.77354209687114	-2.12144241455393

H	3.22353915939026	-9.56271338286741	1.54940328034443
H	6.65092212040740	-2.52297575938920	0.02770844094275
H	5.05110334076333	-0.45634751590313	3.51914328509980
H	4.22056201502862	-2.05600703522488	3.65798458579033
H	2.59185664567661	-0.26844764746965	3.79798054029926
H	4.45376048358680	2.59339958360008	0.70695789489721
H	5.07136484116136	3.35381645402306	2.21961720494162
H	2.73525339840952	4.19763888609328	2.76763076369937
H	2.48136520663158	3.65827098009923	-0.29208482076127
H	1.39201765027021	4.76252786339840	0.76817759160086
H	-1.19752604858828	-0.96534950262162	2.75903384559159
H	0.14865837568103	0.24998320012365	2.91298943865287
H	0.58618224756592	-0.55386620540051	5.24037316714449
H	-3.69665650197518	-2.73433680544540	5.33682362864563
H	-2.54268910402223	-3.95044585826748	5.94921975763150
H	-4.34731655672013	-4.95228060970090	4.38291574123097
H	-3.29233083447424	-5.53247013969213	2.22309939187804
H	-1.91611422028423	-4.27557756076359	2.55556092338246
H	5.40765822871117	-0.61853738797631	-1.00873115180630
H	7.03010764739747	-0.76987253561935	-1.75819844620347
H	6.72755795398393	0.51881245761680	-0.54592900839971
H	8.67858349172280	-2.09713635647672	1.44870521864995
H	8.70393840331686	-0.37686852389165	0.92615575447881
H	9.02280078433239	-1.68422112883930	-0.26321477983616
H	-1.69245748170501	-1.11317491725960	5.76651003635245
H	-0.65622473738441	-2.53437146624877	6.15593363709535
H	3.35999107981903	0.50955960969709	0.89851703400547
H	2.04470205483437	1.21211296848113	1.87183910697706

III-SR

92

Coordinates from ORCA-job 3-SR

C	5.42854835575558	-0.49699717048177	-2.26941694483431
C	4.42659904093718	-1.34515748775516	-1.76665667120762
C	4.21632340612354	-1.47776647108421	-0.35588642340740
C	5.09158360830475	-0.73526627230160	0.49595204583531
C	6.09335903091768	0.10591422862784	-0.00436247755036
C	6.25288358339973	0.22649640486587	-1.39411472118806
C	3.62985123741707	-2.22156221834047	-2.70366557775635
N	2.14444003047855	-2.10191865551946	-2.69545818951301
C	1.67547796907765	-0.72970541033721	-2.98266764499715
C	1.49866090780622	0.10033809540324	-1.71191448709898
O	0.64110958974191	-0.57302042395093	-0.77442444866757
C	-0.73986295724659	-0.18550312495561	-0.79406853379246
O	3.25785213314930	-2.23176167939639	0.11962316429392
Y	1.20677131336632	-2.88379269076375	-0.23851224707714
O	-0.17540696242973	-2.35839776388979	1.43461106437983
C	0.05417262935571	-3.23953810004166	2.38102993198347

O	-0.98830111839502	-4.22337964622481	2.64004501216136
C	-1.22165445362060	-3.66711310914301	3.96070423485824
C	-1.39851301278937	-4.70460817391604	5.05077341312983
Cl	4.88424060243966	-0.89088404495298	2.22522137855904
Cl	7.49512934863508	1.28158732320373	-2.03571899743562
C	1.63253088915767	-3.09157148650162	-3.69710444340879
C	0.14760547162944	-3.08110293051239	-3.95482740931714
C	-0.73651504070167	-3.36194802609675	-2.86500332391838
C	-2.13470360131032	-3.40478761215666	-3.16384917514987
C	-2.63003878515974	-3.19302596295521	-4.45633701677863
C	-1.73030182458979	-2.92101696507111	-5.50003297101126
C	-0.35151297679196	-2.86297778601895	-5.25224924798292
Cl	-3.24483624205733	-3.72791571966300	-1.85821520294188
O	-0.28068082044390	-3.55265442713858	-1.65264433956706
Cl	-2.33907257647894	-2.65075054363831	-7.12061792478291
O	2.22351074307241	-5.05733685846382	-0.52462978227280
C	2.45081959060267	-6.03644390704793	0.20224666866431
C	1.74282782844777	-6.31320103638698	1.50583273568117
C	1.80451343132785	-5.12834359801115	2.49207122292759
C	3.22754742049529	-4.75972416680555	2.92368529638136
O	3.87621761571191	-5.90824849286768	3.43603462169561
C	5.23884132046667	-5.67587109864202	3.79516114837882
C	5.39174645123966	-4.81088486038771	5.01926177314735
C	5.97378337184837	-3.59907552326529	5.02498915331264
O	1.26137267817385	-3.96449543483732	1.87867803532594
O	3.35998049705134	-6.95566733061430	-0.10817028395831
C	4.14619344313537	-6.79092469134488	-1.34135628899631
C	5.33069109290738	-5.87570036486676	-1.05212206467298
C	4.53306553246887	-8.19439545222598	-1.77942834445273
C	0.05886300430941	-2.81903892697251	3.87399402840937
O	-0.21388562275488	-5.42921225207873	5.32442245061122
C	-0.41120798262851	-6.36300284930152	6.36429584085899
C	0.81425331424409	-7.15578457297607	6.70153335966433
C	2.01783442629032	-7.08486603945504	6.11113317601152
H	3.84605490202834	-3.28674603526397	-2.46308383972604
H	4.00054586732654	-2.05149747280784	-3.74490318300965
H	1.93500630511949	-4.09225508994723	-3.31447446641950
H	2.16544582961355	-2.94477305159558	-4.66835742499269
H	0.69550907070828	-0.81188057031145	-3.49577040352929
H	2.36276871846573	-0.19270528540795	-3.68075778746531
H	1.07283163691836	1.09639352053188	-1.96039669071420
H	2.46413636209609	0.26472731171397	-1.19603799925529
H	-1.21031061671666	-0.40431686283933	-1.77704618461029
H	-0.83084228803525	0.89838405281449	-0.56677663401513
H	-1.23816820808352	-0.77396513051234	-0.00178889383056
H	6.73930726926072	0.66501248102953	0.68565657124683
H	5.58078776230600	-0.40544251305999	-3.35554478581145
H	0.33967979932127	-2.65164518643771	-6.08212736986900
H	-3.71123948031171	-3.23505703766172	-4.64410639983746

H	3.47663679647863	-6.31736868167924	-2.08925009624282
H	2.17703934785060	-7.21295872362713	1.97777178580898
H	0.67309546851476	-6.50287019847547	1.27606057721225
H	1.18157886565534	-5.40262975031966	3.37017979966177
H	5.79267218367766	-5.22309619828166	2.93636285295380
H	5.66345293819513	-6.68527633777483	3.98205542644231
H	4.96965117359889	-5.22449267192285	5.95368305861040
H	6.37809927760524	-3.14916677287061	4.10180567531599
H	6.06103476408147	-3.00475710291153	5.94847777392267
H	-0.02930794701873	-1.73004215559936	4.03802873981090
H	0.89157867973025	-3.24165187286733	4.46655649058001
H	-2.14907263853274	-3.04723080337674	3.95463431073061
H	-1.23944632080473	-7.07350085567444	6.09966210076305
H	-0.76854982546430	-5.83945098585437	7.29130883161873
H	0.65601405346330	-7.86523917940001	7.53449119369096
H	2.84229202425447	-7.73128751618332	6.45106427922812
H	2.23510883350837	-6.40756964709563	5.27279522861096
H	4.99393568403887	-4.87273950448117	-0.72380625297299
H	5.94088882657854	-5.74845665350754	-1.96869876099623
H	5.97873949977645	-6.31054805529647	-0.26436779545419
H	3.63538331986020	-8.82032923521187	-1.94878911523070
H	5.16564458671898	-8.68770041521964	-1.01430751709232
H	5.10635533237069	-8.14783322230962	-2.72624349898230
H	3.78206018362042	-4.33610793982520	2.04916873385201
H	3.17082444587500	-3.93928693523052	3.67659944346694
H	-2.22044988347755	-5.39899746016329	4.74287079409052
H	-1.75228953226038	-4.17878894782725	5.97449685990637

III-SS-TS

92

Coordinates from ORCA-job 3-SS-ts

C	1.15774783210750	-2.26266328247324	-2.71307637623874
C	1.84189543222949	-3.35209762776925	-3.34412380466351
C	1.57081461801502	-3.72867088976677	-4.66989381209260
C	0.59860495450019	-3.04295933197116	-5.41352887675830
C	-0.10413432853885	-1.97230712998704	-4.83827638517903
C	0.17458165489455	-1.59782220513304	-3.51698049756567
C	2.93190837640412	-4.02540782874774	-2.55786125222720
N	2.56377554819271	-4.67017079441695	-1.26697793497281
C	1.60186815704945	-5.77405075283350	-1.41061497266899
C	0.16449736387644	-5.32837455435239	-1.66198477535705
O	-0.21290187651867	-4.31650142519848	-0.71647965077949
C	-1.53718547928667	-3.80681543031675	-0.93576143650293
Cl	0.26101305363726	-3.51696080037876	-7.06636239537493
Cl	-0.72317110208563	-0.27142052132302	-2.81163240842004
O	1.42528661062874	-1.92505438814474	-1.48135310599371
Y	1.34850366468675	-2.87765479157446	0.54510656243759
O	1.10075436919838	-1.79400788187746	2.69530781675284

C	0.05210280461086	-2.14534216067363	3.61587023721107
C	-0.23618592573005	-3.63087288173202	3.59169488434516
O	-0.45232319156997	-4.05756789566733	2.23233142673938
C	-0.72211440296461	-5.45834967880339	2.16312534193469
C	-2.16361973238989	-5.82883598614024	2.39235025408257
C	-3.19795455141686	-4.97436324401291	2.46946764663539
C	3.85446644824128	-5.13860808703702	-0.68209160081950
C	3.79844497486009	-6.01502695583063	0.53970049438065
C	4.47141493201556	-7.24887072383739	0.53915319650797
C	4.54656747302760	-8.01924642227966	1.70760773658729
C	3.96126442161469	-7.55304220674050	2.89393075998584
C	3.28608834497059	-6.32612346113988	2.88891281221248
C	3.14793840309919	-5.51539678627759	1.71556141380349
O	2.47693728045138	-4.39372528560580	1.69550269317587
Cl	2.60696291720166	-5.76116194474693	4.40206995970348
Cl	5.38279496867252	-9.55777332855715	1.69473853948208
O	3.15432830327975	-1.39979942260903	0.69625154282803
C	3.58658378794238	-0.32381279125843	1.13272589571438
C	2.82946243203435	0.62598163815795	2.02199590445841
C	1.45457091122971	1.16790671525076	1.51552697027306
C	1.31768224774954	1.25532842838038	-0.00912401236992
O	2.45937546412524	1.98730155403982	-0.45045828600606
C	2.42704952107943	2.30076712132488	-1.84192713404229
C	1.50703631022931	3.45301904953931	-2.15200814866506
C	0.47530624736963	3.40204838084129	-3.01230646354895
O	-0.16975106213170	-1.16304071943486	0.73369099588165
C	-0.06524559372155	-0.72947105381496	1.93762090235233
O	0.33896180236299	0.56419055673755	2.18520969020921
O	4.82980210151463	0.08018137185770	0.88763483626208
C	5.68482234822634	-0.74506546195670	0.02486715638760
C	5.36556305524374	-0.43364527762648	-1.43330283517744
C	7.11538550485165	-0.42943157777118	0.43256703391246
C	-1.02309703245183	-1.20268660343663	3.04769360729369
H	3.69787231165291	-3.26187018988144	-2.29649175739581
H	3.43891275665344	-4.78075248877103	-3.20905141871342
H	4.42925398320132	-4.21483317506767	-0.44291203491710
H	4.43900933337338	-5.67756744743891	-1.46797563167672
H	1.64479676401451	-6.36404681674703	-0.47185119062295
H	1.88550394575214	-6.47733125524849	-2.23537554562802
H	-0.50953468495120	-6.20983871512345	-1.54465237375599
H	0.02676327164576	-4.92812661684776	-2.68785696501590
H	-2.29257133910703	-4.59514307615906	-0.72710772135807
H	-1.64092848366244	-3.44742133177184	-1.98176581719051
H	-1.67670459375666	-2.95473679120202	-0.24512689182123
H	-0.86788973589922	-1.43071570883285	-5.41240174675044
H	2.12111411446379	-4.56241542711620	-5.13223542073314
H	4.95693666812713	-7.61003676574599	-0.38008393703069
H	4.02959262899674	-8.13762900588770	3.82103462094676
H	5.44142406300276	-1.80570753198501	0.24580353815473

H	3.49946864480395	1.47844936769962	2.23016731283493
H	2.63010691783707	0.08275028247516	2.96916469260657
H	1.41302202203005	2.21036320149804	1.89030995212416
H	2.14674082585624	1.40498337003319	-2.44465381024022
H	3.47289558032992	2.57517115822252	-2.10339223674210
H	1.72679654772389	4.38964197258185	-1.60660616861724
H	0.22234491834833	2.47198179951303	-3.54902629366676
H	-0.15645890907399	4.28344640666864	-3.20747391876487
H	-1.91664666855156	-1.69861203958355	2.62460215904648
H	-1.32423556775904	-0.38548950921864	3.72797128308751
H	0.34050984843506	-1.88694240309002	4.66159797430443
H	-0.06212248147149	-6.00336391725841	2.87798169350927
H	-0.41772385650069	-5.78927131868205	1.14772901729635
H	-2.34297066118268	-6.91606880470530	2.48477236654367
H	-4.22592122213861	-5.33335300740608	2.62915688070348
H	-3.04651643879467	-3.88691753657988	2.37711493157290
H	4.30919655153658	-0.66852492638716	-1.66894335386716
H	6.01312485281362	-1.04100204096165	-2.09734110955750
H	5.55075652540395	0.63703489082478	-1.65332488530366
H	7.28168805878516	-0.65063683116987	1.50488887332567
H	7.35034741364511	0.63919011014842	0.25394475773499
H	7.82055025470064	-1.04387981062443	-0.16117811352263
H	-1.13521158351694	-3.85692691657973	4.20911064783356
H	0.63329221343260	-4.18794626681817	3.99995277400564
H	1.27148961199165	0.26005511791247	-0.49922270437179
H	0.36741923519004	1.78651077243911	-0.24687857449364

III-SR-TS

92

Coordinates from ORCA-job 3-SR-ts

C	-1.29147063650167	-3.02250978206137	-4.58683821757555
C	-0.58783995242557	-3.15217354047884	-3.37606856799946
C	-1.26877396865098	-3.09214133768368	-2.11884611512885
C	-2.68201260805636	-2.87695741889143	-2.16544994551073
C	-3.38446965894785	-2.75235406992737	-3.36976705495383
C	-2.68052294957326	-2.82901331235270	-4.58289461623739
C	0.89682487701180	-3.41035779391426	-3.37285817342837
N	1.73632535883775	-2.42599241015774	-2.61897345313460
Y	1.22399631083808	-2.78374755280126	0.05712425173905
O	2.41740583206557	-4.86576528023986	0.32938597178206
C	2.89248255034791	-5.55480756162252	1.24424129759555
O	3.94378945034568	-6.35482902359491	1.05231225777322
C	4.59589668005633	-6.38165170154570	-0.26410188340366
C	5.13077163722678	-7.79475898931100	-0.43911566929399
O	-0.62334404476632	-3.21924247577386	-0.98974734933355
Cl	-3.55161705833540	-2.76224995655407	-0.65167466246622
Cl	-3.54629996082051	-2.67430595634629	-6.09749072930905
C	3.15761423122642	-2.79216757066773	-2.87834837950955

C	4.24175766210420	-1.92980760215906	-2.27812428219954
C	5.24799901091963	-1.38910655300927	-3.09745264638382
C	6.33717712582346	-0.70968067988091	-2.53103163396164
C	6.44274550399183	-0.57382742725242	-1.13736970467917
C	5.43681910693269	-1.10614618252483	-0.32150492463723
C	4.29099476528393	-1.77821903588018	-0.85370258399470
O	3.33674427986246	-2.23562875405505	-0.09022099375867
Cl	5.57133646203684	-0.96293100171729	1.41536870597996
Cl	7.58055144713459	-0.03552311399563	-3.56509470561779
C	1.42463160806711	-1.02883605309839	-2.99495129202015
C	1.58684643816905	-0.05826732770885	-1.82500265158178
O	0.82628293105016	-0.49372261865011	-0.68608791990944
C	-0.46548498318391	0.10096584249895	-0.52981836976728
O	0.64817331841886	-1.73329463989224	1.98719474290288
C	0.73806467713923	-2.81066683669028	2.69135985133411
C	-0.39191139377530	-3.16686258677140	3.66768061219350
C	-1.09053844313379	-3.92948745360232	2.52403485394587
C	-1.75130263040096	-5.26062608669547	2.82725428781960
O	-0.90805604595615	-6.07337498212973	3.62271699975693
C	-1.42920718208372	-7.36358080451347	3.84511216939696
C	-0.58357004096941	-8.15333129742199	4.79926474748064
C	0.48205781355306	-7.68963860734209	5.47213031501447
O	0.10356455666662	-4.08519622911751	1.73421320500047
O	2.08011920223431	-3.14210931489027	2.89333852591510
C	2.54290350962076	-4.34619834997528	3.50558820727836
C	4.01335511812453	-4.03580376997879	3.80920373121350
O	4.60917096691098	-5.16105074804379	4.42159402749416
C	6.03288698840848	-5.11001479555502	4.43233408251567
C	6.58673818508121	-4.02267017341313	5.31631520404507
C	7.32676317444561	-2.99032986478889	4.87661837605448
C	2.36387159393022	-5.62710434284824	2.65374241008338
C	5.66548946072457	-5.29663419769884	-0.29903750469922
H	3.27625351557625	-3.83252953617355	-2.49725582097104
H	3.32201596612130	-2.84223522121580	-3.98326601814917
H	1.10397335393902	-4.40578672580785	-2.91689268607014
H	1.25199866789072	-3.46970682462899	-4.43070396951411
H	0.37057824865591	-1.00116806837421	-3.33806638967463
H	2.05328254036521	-0.68064686869713	-3.84930127703584
H	1.25968597556781	0.96007054305598	-2.12717733799096
H	2.64019106412716	0.00896853993224	-1.49434574396552
H	-1.13082191461666	-0.12892438996399	-1.39004047348613
H	-0.36576880363445	1.20173864123027	-0.41424840208164
H	-0.89968225182523	-0.32349151003945	0.39361618218029
H	7.29995241296951	-0.05567110122174	-0.68707221018156
H	5.19518392661241	-1.51058836039023	-4.19009604622081
H	-0.75457231823878	-3.07448443350723	-5.54607200064730
H	-4.47082154209757	-2.59193929357675	-3.36073038150173
H	3.81245330552334	-6.16373219227224	-1.01933863516157
H	2.89421667228752	-6.43570813201660	3.18963847098881

H	1.28154162877829	-5.85601412438749	2.59771689088953
H	2.00400226465631	-4.52632194151288	4.46337265501383
H	6.42539570451811	-4.98863210679016	3.39197713652989
H	6.35456800297567	-6.10679755909751	4.80309258645008
H	6.33208462377478	-4.10204012213804	6.38928439069847
H	7.57137553728895	-2.87365697526103	3.80655118560212
H	7.71022631243456	-2.21839068331299	5.56250260773353
H	-0.90191707284121	-2.27627875871444	4.08086761624151
H	-0.08180728354533	-3.85292530387821	4.47815421394767
H	-1.84217172693699	-3.29939165807009	1.99375657027549
H	-1.52612849989026	-7.92448887530414	2.87829107701397
H	-2.47377472081022	-7.30193956923090	4.25197916042408
H	-0.91137330771897	-9.19964216768726	4.93541228833896
H	1.04688352974297	-8.33576860445149	6.16101316596627
H	0.81901215128600	-6.64861095863878	5.35444106741987
H	5.22336034219945	-4.29585367835679	-0.13047086254094
H	6.16568629324326	-5.28738519728159	-1.28816625874203
H	6.43705122935437	-5.48270200650276	0.47569222661351
H	4.31456546167053	-8.54117560871724	-0.38096635705115
H	5.87938868473262	-8.03313604955004	0.34313708661253
H	5.62062449939263	-7.89232681357157	-1.42809552945656
H	4.52852263443101	-3.76440843330072	2.85481046222050
H	4.05885119322958	-3.12938780792835	4.45597897957301
H	-1.98856195996252	-5.76109962935844	1.85656032034371
H	-2.72467761823668	-5.07564611056341	3.34846225554544

IV-SS

92

Coordinates from ORCA-job 4-SS

C	2.36265705133566	-3.78080719188721	-5.23732816920112
C	2.70355853769520	-3.64616767354429	-3.88075169373556
C	2.50573578244567	-2.40820888380124	-3.18505214948488
C	1.96176534066934	-1.32833550289209	-3.94880451339696
C	1.62211576246283	-1.46156816905637	-5.30181871629297
C	1.82152623608123	-2.69480901329916	-5.94201744492218
C	3.37803668212762	-4.77160277507295	-3.13758232723125
N	2.67715157226828	-5.33624227739883	-1.94467656151816
C	1.32965294913185	-5.84680405155751	-2.26739501867619
C	0.25916436181957	-4.77328540316066	-2.10773510446923
O	0.28633282978679	-4.26218539923992	-0.76245754946373
C	-0.69888150222396	-4.83605703291665	0.11120137534050
O	2.80065485902587	-2.29962435929582	-1.91440028033808
Y	2.42686342699474	-3.33432205430476	-0.01077555196332
O	0.99000460125123	-1.13355413507221	0.39839319989268
C	1.16493062380827	-0.72499936557480	1.54090699811755
O	1.45498250430024	-3.41895966830196	1.89220939278980
C	1.11607228433766	-2.76017829504652	3.03465644829324
C	0.16287062353141	-3.56234997485914	3.93447427110849

Cl	1.70548795175360	0.20470670656863	-3.15236428822225
Cl	1.39564830156356	-2.87371257193650	-7.63285878823335
C	3.53707318996145	-6.43332064166582	-1.40855355617813
C	3.23756792272545	-6.84576225796264	0.00819952634345
C	3.57103199001766	-5.89102938258483	1.02475179929453
C	3.41186381910245	-6.32104175430851	2.37844692801060
C	2.92914402827217	-7.59412712051621	2.70690872607492
C	2.59341515847734	-8.49036759672682	1.67894248496690
C	2.75575806605738	-8.12458355535357	0.33411568064737
Cl	3.85552495184806	-5.22382285565018	3.66588083528025
O	4.00154032937101	-4.69138694737976	0.69347186531313
Cl	1.97778063258926	-10.08041922646773	2.08525765883620
O	4.04722345409744	-1.74302137440561	0.76616713902579
C	4.51974043126982	-0.85151186535044	1.47331782968455
C	4.02533128979116	-0.55254199997379	2.87366064093148
C	2.86010435640890	0.46895766192162	2.87319000951772
C	3.33717041046732	1.92137826759364	2.83873185226826
O	4.08706764457211	2.14398672486839	4.01422730405464
C	4.66315809937392	3.44470902093967	4.09918266848414
C	3.64521575515427	4.53282461403375	4.31788559023080
C	3.53166560098761	5.63866473263975	3.56297210061255
O	2.05474003919990	0.30080034267387	1.69659873993289
O	5.50138247478775	-0.05100508738106	1.07520464262246
C	6.05678753688210	-0.23797260871081	-0.28477713010279
C	5.16673958084094	0.46052555053505	-1.30272037343041
C	7.47851988924812	0.29596624745426	-0.21549104109243
C	0.47907931326925	-1.33942517730241	2.72235789817464
O	-1.09887289203318	-3.71062935687814	3.31069123059972
C	-1.98133143902957	-4.54765628494299	4.01956062860594
C	-3.33784097647577	-4.59631217404308	3.38107769285743
C	-3.72768908145062	-3.87547784605756	2.31668369454473
H	4.35877934894509	-4.40715440667612	-2.76020869143232
H	3.59133050714523	-5.59934602552717	-3.85747289719038
H	4.57704456197785	-6.04720370791751	-1.43537263130040
H	3.49394003225644	-7.31697388180282	-2.09001731353423
H	1.10217345411080	-6.67186251954761	-1.56056273420262
H	1.28627651206385	-6.27736050502962	-3.29771850673015
H	-0.74700423975830	-5.18750094418441	-2.33029404501415
H	0.43193360457538	-3.91883011227017	-2.78954575885952
H	-0.58299528027046	-5.94094909989581	0.16682392001036
H	-1.71803848356917	-4.58926254358363	-0.25566603765645
H	-0.53747789134369	-4.39808587840030	1.11233323945673
H	1.20071861115122	-0.60741539288714	-5.84855850596648
H	2.52806308640927	-4.73657576935485	-5.75737723211174
H	2.52181329643741	-8.85004402915699	-0.45998329183043
H	2.81663231353818	-7.88469349202286	3.76004052022940
H	6.05465610200227	-1.33143108638050	-0.47427863085232
H	4.83748603598465	-0.13357127067122	3.49834560724897
H	3.69417423436483	-1.51555040338365	3.30653508129211

H	2.26232567297118	0.32518901680823	3.79921880328210
H	5.27736516589192	3.66625954096775	3.19200874685971
H	5.35367001865052	3.39295119462082	4.96855251217607
H	2.96819373658035	4.37823043714556	5.17831135708381
H	4.19282779869033	5.81266864572997	2.69659605045421
H	2.78563744391212	6.41784671909915	3.78467539522680
H	-0.56895349757159	-1.52245480722055	2.41595378537626
H	0.48268244491575	-0.69985241037086	3.62659925697466
H	2.01375812614065	-2.57586082244935	3.68903273056537
H	-2.09223804887664	-4.19789221438105	5.08106729093411
H	-1.56646044749104	-5.58709503498892	4.09765525335447
H	-4.04459936744532	-5.29149638749504	3.86905044730542
H	-4.74764212849110	-3.96405609984206	1.91248442489021
H	-3.03700320541347	-3.17555902809522	1.82215295367243
H	4.15894026766221	0.00496366887250	-1.35046713542713
H	5.61827344620724	0.36208375982434	-2.31039547621362
H	5.07738976056228	1.54214570428120	-1.07326081055746
H	8.06680121535506	-0.22838338901884	0.56278723304608
H	7.48462485660878	1.38172199856754	0.00990140497464
H	7.98138022803837	0.14387116361504	-1.19070507526668
H	0.04905950763499	-3.05194445744129	4.92547543902468
H	0.63950139862192	-4.55486676278365	4.11699911570081
H	3.95303184550439	2.09668644884768	1.92291386336475
H	2.44491559936919	2.58713322705184	2.77261374713761

IV-SR

92

Coordinates from ORCA-job 4-SR

C	-1.55154109253928	-2.96876591977260	-4.66307496997810
C	-0.87547153248476	-3.12227698967390	-3.43934331340665
C	-1.55728587036093	-2.93891004572743	-2.19380781047019
C	-2.93872371370342	-2.57310792078599	-2.26703471611125
C	-3.61322630386851	-2.42442987021245	-3.48430376788130
C	-2.91177021458203	-2.62785077777589	-4.68445642461414
C	0.57519879789974	-3.52954331659354	-3.40737239676224
N	1.49748002688508	-2.61466017698524	-2.66042363809609
Y	0.95586784295869	-2.89987598556524	-0.01798172367622
O	2.45468180002194	-4.89237987520159	0.14761966370868
C	3.08284117461854	-5.30717908749956	1.12912730339395
O	4.36105438413123	-5.68987703831809	1.05862220716459
C	5.08664518530979	-5.56025484830561	-0.21406050964713
C	5.00264089185971	-6.88998205415570	-0.95320377364912
O	-0.94084593291843	-3.09190040907732	-1.05369678708931
Cl	-3.79865504328479	-2.30379573919129	-0.76803601208830
Cl	-3.74364352760518	-2.44501997994661	-6.21530121993309
C	2.88083671043681	-3.11372841893625	-2.89430236065965
C	4.03768734926686	-2.31851684353641	-2.33356900067588
C	5.11383403648455	-1.98548709640440	-3.17587829229427

C	6.26945117105843	-1.38246873352705	-2.65797010334637
C	6.37110475127504	-1.11317147853443	-1.28374198990457
C	5.29697884249763	-1.43522286742604	-0.44634194430207
C	4.08107432816217	-2.02227097764894	-0.92831670391469
O	3.07403082507190	-2.26864856478514	-0.14182653313438
Cl	5.43484758148914	-1.13081681334037	1.27175051331298
Cl	7.59685022668932	-0.97107437753113	-3.72509716443899
C	1.31720145838753	-1.19750078810858	-3.05525925213034
C	1.48964926081712	-0.22343219692725	-1.88745505171917
O	0.63684697627637	-0.57522082318123	-0.78391749684425
C	-0.63021039038007	0.08584178731732	-0.76111152884991
O	0.77809208096164	-1.64205608220035	2.07991761618791
C	0.99864643233621	-2.58567164357682	2.85666965390710
C	-0.11699523506784	-3.24501226665245	3.61970862498468
C	-0.88804304355986	-3.96668444756122	2.44956528237927
C	-1.60891789529983	-5.22559539802088	2.93530003370045
O	-0.70778236652514	-6.08484036828155	3.61523950457902
C	-1.26001097106154	-7.34552230318077	3.91026188588262
C	-0.34520910508069	-8.18162677834004	4.75453676128194
C	0.82746781446742	-7.78650107494705	5.27609600189896
O	0.03267113467719	-4.24137566044827	1.44534792565767
O	2.26781676302325	-3.02950166827145	2.89613359497456
C	2.71261721306426	-4.27576148195995	3.47995910833402
C	4.16733709265571	-4.01645983586803	3.87872881250481
O	4.64115786581334	-5.18749500616319	4.51448822507970
C	6.02555552082430	-5.17311878839740	4.80754938471854
C	6.39726894592090	-4.45391289845865	6.08098781664637
C	5.52675059091958	-4.05115752526205	7.02092756506668
C	2.51507634880037	-5.47034621005116	2.52347124660628
C	6.50060681972138	-5.12811264791465	0.14284619381170
H	2.90811081922595	-4.14296451033685	-2.46877999403046
H	3.04305976297945	-3.22854409942500	-3.99461291563218
H	0.67639659697742	-4.53053684195879	-2.92754483469587
H	0.93743786517860	-3.64784796054664	-4.45770210855677
H	0.29006166188427	-1.09088530103228	-3.45894412179460
H	2.01744854231224	-0.90758022385704	-3.87396267175171
H	1.25789435708121	0.81061233564448	-2.22391108718247
H	2.52297142692517	-0.22831752856843	-1.49683238051861
H	-1.20093350920792	-0.08719496059033	-1.69866832359414
H	-0.48810187285886	1.17703688980144	-0.60323448031820
H	-1.20864083152429	-0.33396856333225	0.08166160290275
H	7.27730513093624	-0.65445008435603	-0.86601116852268
H	5.06069228796651	-2.21290379841844	-4.25152418693436
H	-1.01541828344150	-3.11646196131023	-5.61274931504393
H	-4.67610101925575	-2.14842903738607	-3.49562946200718
H	4.58081205011051	-4.76538067177434	-0.79700293698225
H	3.02472479448000	-6.32431983465231	3.01072361711658
H	1.43053415219898	-5.66742423522739	2.41991219419406
H	2.13103494849480	-4.49387447813665	4.40054575204741

H	6.60332497434774	-4.74711894272586	3.94977964222920
H	6.33912353014075	-6.23944242763521	4.88693275409414
H	7.48068058863379	-4.28537847212008	6.22316486160382
H	4.44540547180985	-4.22555993323992	6.90040417573760
H	5.86379048980778	-3.54324591288698	7.93711759079786
H	-0.72612107509899	-2.46638006446325	4.12011627872875
H	0.23070549795131	-3.98126704875227	4.36645892516037
H	-1.69979023605337	-3.27529040677898	2.09746177963899
H	-1.50679049406663	-7.90077299948032	2.96719424023752
H	-2.24073480119265	-7.23308330897365	4.44583865762273
H	-0.71610432300587	-9.20493922012465	4.94493382228802
H	1.43607337472025	-8.46551767445805	5.89227398137624
H	1.21321257360991	-6.77076717040795	5.10272283033953
H	6.49330296290109	-4.15303502957329	0.66837005619460
H	7.09882715764406	-5.00831753824596	-0.78198240317907
H	6.99795987691824	-5.88259693538853	0.78599537201688
H	3.95101520504850	-7.15486553058631	-1.17961393624324
H	5.45200441129013	-7.70618688710141	-0.35180381012354
H	5.55301458410096	-6.82386830989987	-1.91305780452463
H	4.77183945571120	-3.76672057854764	2.97518944245346
H	4.19986050220533	-3.12868432055593	4.55247387470687
H	-2.03492020197147	-5.73057507617148	2.03592285488681
H	-2.46145241237580	-4.94966103350530	3.60718219509689

IV-SS-TS

92

Coordinates from ORCA-job 4-SS-ts

C	0.88154530912720	-4.31286951831318	-5.37648174395583
C	1.44416874517346	-3.85367464483842	-4.17372513392805
C	0.85480590300326	-2.77273118961042	-3.44313760669280
C	-0.34981646410844	-2.22176278936672	-3.98093225285978
C	-0.91538059957166	-2.67953872244427	-5.17841115086307
C	-0.29019506499346	-3.72491394463116	-5.87716124255403
C	2.71474304902397	-4.45398710868695	-3.63209752366416
N	2.65232026721160	-5.09332674603499	-2.27996139292734
C	1.65351228846667	-6.17613495249874	-2.19310823650174
C	0.23191290194856	-5.69903309833304	-1.93386662849293
O	0.23315154340285	-4.83621735658311	-0.78776506963682
C	-1.08827154282067	-4.51623016799644	-0.32340487052605
O	1.38137601653472	-2.35389759660941	-2.32059571197035
Y	1.99495632805601	-3.18027767457384	-0.39707799712743
O	1.29518573460336	-0.96330084048883	0.23754374089293
C	1.33275331081583	-0.54791630631277	1.39862303988345
O	1.15528090059141	-3.39076600529737	1.53928087131082
C	0.96399834397846	-2.72833209646077	2.71951811474918
C	-0.11336725248961	-3.39635871048871	3.59002913482262
Cl	-1.15077405856886	-0.95562404984908	-3.08345092628088
Cl	-0.98429417942134	-4.30007585863573	-7.37988054411172

C	4.01694660886796	-5.64433112637577	-2.01453678065526
C	4.26305181226942	-6.12320314291328	-0.60924175940431
C	4.27624903187661	-5.12049674821161	0.41277208940490
C	4.60604324269057	-5.56088191283625	1.73093047523847
C	4.89489593078727	-6.89897984687013	2.02622249338060
C	4.86293995479576	-7.85135118172886	0.99496112620560
C	4.55275341841379	-7.46653508079565	-0.31831650363764
Cl	4.65659379611169	-4.37833656394482	3.02331033543383
O	4.00284451097801	-3.86723998098836	0.12297520957926
Cl	5.21796305807053	-9.52835788990327	1.35494441656220
O	4.12513357861617	-1.13227051717740	1.06972991739694
C	4.56792666207801	-0.73549518435068	2.13599884647354
C	3.70800149382215	-0.20522859730049	3.27741480053868
C	2.67769424388202	0.86554349165036	2.87584681463062
C	3.30379489912974	2.24732849997955	2.67531157731706
O	3.82843369305269	2.65528275190402	3.92014448280939
C	4.51087353144876	3.90558962881667	3.88184896196429
C	3.59188475858002	5.07914560393366	3.66581351257334
C	3.74740221598957	6.00714324857017	2.70646966556297
O	2.04392369694873	0.57279519852393	1.61613479523523
O	5.87006912494684	-0.75882520936812	2.47187800589690
C	6.79162287996852	-1.40000052729340	1.52362422401926
C	7.30825570859674	-0.34787700653560	0.54930688957294
C	7.87307306797937	-2.05872402282116	2.36606568167144
C	0.56738569984086	-1.21583215628007	2.50490937521169
O	-1.37616265507085	-3.28261282920304	2.96091300018094
C	-2.41227247455458	-3.94872661848890	3.64119554057275
C	-3.73377459731584	-3.76898041166783	2.95442025116668
C	-3.95085837391467	-3.02680514091249	1.85599745457532
H	3.48427169773256	-3.65465284455991	-3.54900110852353
H	3.10100083395574	-5.20341008945083	-4.36542374364282
H	4.72600458274359	-4.81771809677367	-2.23164816490199
H	4.23449952306666	-6.46496446854069	-2.74070955492442
H	1.95750050974806	-6.82729581919683	-1.34759107688324
H	1.65394633604595	-6.81154292816014	-3.11354577359240
H	-0.40535734033844	-6.58635327328462	-1.71448315104836
H	-0.20810135890685	-5.16887100883392	-2.80439477127868
H	-1.66592890182227	-5.45170931174505	-0.16040387208732
H	-1.61882245762378	-3.87922330018488	-1.06510763656276
H	-0.96829913771227	-3.98622751608750	0.63969907862542
H	-1.84107738095707	-2.22638827587508	-5.55770758516267
H	1.35468943755631	-5.13774380614317	-5.93050979209522
H	4.55023890762982	-8.22089410520145	-1.11972177977809
H	5.14009335416447	-7.19581400502083	3.05468435364224
H	6.20269478619417	-2.16465963131242	0.97578274830565
H	4.34467838487869	0.22188540111667	4.07504543730510
H	3.19048218642598	-1.08992205478672	3.70580150921353
H	1.91918674765233	0.95445169240956	3.68537540079430
H	5.31394587421840	3.89561298264402	3.10441421847970

H	5.00466247645981	3.98961348921280	4.87399109970807
H	2.74613260915495	5.15215264436123	4.37430795995862
H	4.58043262613498	5.95220518893275	1.98464432176970
H	3.05953271777655	6.86170676840891	2.60946360030201
H	-0.49193397573654	-1.22181894927254	2.17250295153191
H	0.61938756630511	-0.66000669554170	3.46098987693862
H	1.89636452653730	-2.74331514715975	3.34870477023394
H	-2.49553269302432	-3.57900143829340	4.69845219902397
H	-2.18702072652201	-5.04423306530937	3.73353035180349
H	-4.57128594292515	-4.30694834428932	3.43410817824522
H	-4.95615820459620	-2.94342250523960	1.41579345047255
H	-3.13014309980536	-2.47984923016746	1.36699903675825
H	6.47568678016316	0.08832124069060	-0.03647378201142
H	8.02014643680576	-0.80861557311498	-0.16482331680923
H	7.83645710710230	0.46612753506032	1.08714903285388
H	7.42935662435010	-2.81457822509032	3.04277687908922
H	8.42023051105662	-1.30965360790971	2.97427206716432
H	8.60265514452374	-2.57192156961557	1.70838794270391
H	-0.13906260207825	-2.92813913396306	4.60760134980647
H	0.17109729674314	-4.46836357899407	3.71665391593329
H	4.10081634453943	2.19202219899264	1.89202628061565
H	2.52046189353358	2.94423110793187	2.29540532897942

IV-SR-TS

92

C	-2.03868765102163	-2.74725633210533	-4.41887671140635
C	-1.30528053968750	-2.85665093544679	-3.22325292159072
C	-1.86856487005645	-2.43244954400181	-1.97605216101833
C	-3.19117932534080	-1.88951489846385	-2.02000697693296
C	-3.92263205031998	-1.78695145706533	-3.20866467063151
C	-3.33853444674533	-2.22080166464164	-4.41040768971529
C	0.06990779093756	-3.47833002723699	-3.22784517236901
N	1.17777998561203	-2.64540750203259	-2.64907250783942
Y	0.82123121095610	-2.63149460451468	-0.06930341262882
O	2.92785144852379	-5.23933929553556	0.21654963039030
C	3.44619181552175	-5.35119139857078	1.31700978917713
O	4.78358970549641	-5.44715386505235	1.50895034843898
C	5.64752551879314	-5.42308967343890	0.32708721545125
C	5.72498685643179	-6.82772441923612	-0.26318984401952
O	-1.19693970208463	-2.52876625061283	-0.85944874920616
Cl	-3.89931179683661	-1.33827673784847	-0.51958924922152
Cl	-4.24061188946055	-2.09576870716112	-5.90631363602640
C	2.45899470217510	-3.37338071484500	-2.91094036099769
C	3.74455421476311	-2.68030704410913	-2.52877665655848
C	4.76950514749498	-2.51376684420056	-3.47580607267403
C	6.00604640161346	-1.96810255659319	-3.09744056118688
C	6.23455599513697	-1.58091610051238	-1.76720559285996

C	5.21030185207767	-1.74058631608216	-0.82554169155687
C	3.93269280976095	-2.28672273377415	-1.16344062573017
O	2.97094469401796	-2.40213330635691	-0.28911864822514
Cl	5.48404002378781	-1.25471447182690	0.83272710458503
Cl	7.27406658209662	-1.76769022610609	-4.28886198138926
C	1.17020166487084	-1.25775964902415	-3.17649444351444
C	1.58165169596248	-0.21043115957791	-2.13623790392841
O	0.78623683860694	-0.30971955213105	-0.93931117047518
C	-0.36600241561762	0.53755098769169	-0.90642511905250
O	0.74112106850508	-1.71397193651380	2.13573260685139
C	0.97211624015250	-2.71291921090948	2.84686042967080
C	-0.15876979994583	-3.52798148523121	3.41762322697055
C	-0.82225563273656	-4.15488824785308	2.13393486139560
C	-1.50352309626965	-5.48951071221036	2.44367150168083
O	-0.62010066032919	-6.35986686663701	3.12975620711968
C	-1.10752964532399	-7.67705597607164	3.23419694386893
C	-0.26031902282290	-8.52488164525871	4.13554752821682
C	0.77442984784664	-8.09718532337699	4.87690260641108
O	0.16023087844417	-4.27414925555988	1.15029378812985
O	2.25363134322936	-3.04844307109908	2.99611126389538
C	2.73775856120017	-4.27809998937690	3.60346436817620
C	4.12949793618321	-3.92020006210918	4.13063616451187
O	4.60625812757566	-5.05228736123431	4.83162813514793
C	5.99469932157689	-5.03902657449417	5.10217650499194
C	6.39840979582185	-4.24419138007469	6.31920615456401
C	5.55028628892947	-3.76087229812108	7.24158993768525
C	2.68719036607614	-5.46792993747968	2.63130702354457
C	6.99066483742937	-4.87399665569099	0.78463272772152
H	2.39440332565429	-4.33565775639006	-2.35260088996728
H	2.50743033702837	-3.63585487404267	-3.99535730499732
H	0.06027422337800	-4.42822821640511	-2.64430103260979
H	0.33044019323236	-3.76028481015725	-4.27610139746940
H	0.13775849395880	-1.03783500811638	-3.51577904179562
H	1.83245626759578	-1.15713922807684	-4.06790275243900
H	1.47653993111773	0.80728155413321	-2.57121361119425
H	2.63426259383753	-0.33508977855813	-1.82365136674958
H	-1.02628211196778	0.36877488906625	-1.78397526087219
H	-0.05350794981022	1.60376111927309	-0.87149609690386
H	-0.93497881135659	0.28935166322263	0.00776394445233
H	7.19919540662666	-1.15174066151117	-1.46498755289056
H	4.61204926523523	-2.82212153587854	-4.52041093108818
H	-1.59640751399333	-3.07911895574214	-5.37030617777843
H	-4.93766128468060	-1.36791604136827	-3.19714500021084
H	5.17937369051918	-4.73666184757612	-0.40783497112639
H	3.12172456713380	-6.31664475785992	3.19807478698812
H	1.63371798551006	-5.69629125370492	2.38313007022872
H	2.09737750821285	-4.53431081388758	4.47406339786015
H	6.56259192852778	-4.67990637750716	4.20850169542129
H	6.29463425229971	-6.10256501691906	5.24641700076375

H	7.48710178378831	-4.08940486284268	6.43535835681977
H	4.46405535528127	-3.92037044429314	7.14774892053299
H	5.91102629755233	-3.19981234293285	8.11690214128185
H	-0.85148916210287	-2.84862455206147	3.95356966047175
H	0.17764203310024	-4.32313815428576	4.10595245899215
H	-1.64792652562400	-3.46934481542572	1.80603164022811
H	-1.17203584035966	-8.15638530699658	2.22226847949697
H	-2.15998151322436	-7.67934629652590	3.62579173817628
H	-0.55963045381532	-9.58804450029850	4.16814045968042
H	1.34012812789776	-8.78830996424890	5.51992340731232
H	1.08595005679152	-7.04202484481741	4.86209405799752
H	6.88122850859152	-3.84746227705036	1.18570614253535
H	7.69101869726510	-4.83159590625741	-0.07313258817879
H	7.43970603494847	-5.52222242290159	1.56532674485815
H	4.72378332150446	-7.17516394688437	-0.58361880779505
H	6.13371384038037	-7.54489630006298	0.47786263293192
H	6.38815715029185	-6.83079732596625	-1.15155894169993
H	4.79795466115804	-3.65610118652930	3.28003840976124
H	4.04422415237244	-3.02266051623558	4.78703194316229
H	-1.81809346904581	-5.92998293790644	1.46779493421632
H	-2.42778237782007	-5.31879839775535	3.05268816375492

V-SS

92

Coordinates from ORCA-job 5-SS

C	4.58511816613193	-8.28271245408862	1.60577651180817
C	4.02584929732796	-7.03932034187437	1.25845436600477
C	3.41333843580916	-6.20963457306083	2.24888220834519
C	3.39816913592291	-6.70490180329815	3.58865753715979
C	3.95801213435235	-7.94041287971031	3.93506012451612
C	4.55225498934553	-8.72761521476800	2.93505580553370
C	4.13014570540812	-6.51968383635934	-0.15313858491211
N	2.84412053974412	-6.19552604315936	-0.85233076068809
Y	1.67249698443360	-4.08942918529152	0.42719564128692
O	2.80825409747867	1.35018839693763	-0.30142632354297
C	3.91941850458294	1.42323790525691	0.19335052837576
O	4.57791838735524	2.58490643365021	0.42707832762346
C	3.89399527259548	3.82275612343253	0.05263674687352
C	4.98396997182349	4.82456590878039	-0.29799268641955
O	2.87940783082413	-5.05464974759298	1.92908725187110
Cl	2.64249718641219	-5.72655789174820	4.82101252184491
Cl	5.25282978862386	-10.27672426341766	3.35528644460405
C	3.20875154311054	-5.80621433280566	-2.24709491455109
C	2.09911594487218	-5.32023604644618	-3.14466895372035
C	1.78584474521098	-5.99553292250285	-4.33716064136103
C	0.78303559234504	-5.50325105636118	-5.18617578881326
C	0.08284697230597	-4.33163062215440	-4.85500672819468
C	0.40016591457419	-3.65757032717133	-3.66855175292575

C	1.41918021688794	-4.11592913720733	-2.77793146431224
O	1.70582094475457	-3.49019087868591	-1.65900975768938
Cl	-0.47911183236303	-2.21054421502600	-3.24044359136703
Cl	0.39884465127253	-6.35227775504833	-6.66885393639092
C	1.90653625155324	-7.33234731193466	-0.78965224994987
C	0.44395193343276	-6.95616784626934	-0.99029096679516
O	0.09457360082270	-5.88122666450503	-0.10048835735688
C	-1.31841095575052	-5.63872718447447	-0.04140453836598
O	2.64696104769767	-2.06594624659229	1.12042214923178
C	2.13529079787737	-1.10398127091232	1.71863053641322
C	0.66759485905618	-0.86118261128899	1.87971494701956
C	-0.16389861304022	-2.11936640435642	2.26974817646565
C	-1.64873730763167	-1.70256133987187	2.37731715937334
O	-2.14579200844520	-0.97618904345568	1.27288817241382
C	-2.49335704072508	-1.73925313799689	0.13171398308146
C	-3.25330504445793	-0.90608619996169	-0.85690633345309
C	-3.62133021706570	0.37226919219237	-0.67243687167336
O	0.03017341611845	-3.16671695000874	1.38104076066737
O	2.89478450022227	-0.16333748160816	2.28289910040758
C	4.33594214248003	-0.21879415350475	2.08710250863396
C	4.91516144184808	0.67178705392584	3.18560881859859
O	6.31998327445981	0.56488581325694	3.10480100533962
C	7.02014445998384	1.41193499575445	4.01005486612873
C	6.86930845370918	0.99933392288048	5.45076074217963
C	6.48335768748568	1.81615979803313	6.44555933579569
C	4.71903835644348	0.22005450389860	0.66143638891748
C	2.98822743653422	4.26532316718536	1.19720147107874
H	3.96229202674000	-4.99393326045719	-2.14487919053291
H	3.72556314093586	-6.66582090262363	-2.74027911528044
H	4.72415395028443	-5.57785549319891	-0.15809319435612
H	4.70416290026918	-7.25822677073169	-0.76392272096558
H	2.01618244478760	-7.78777911927100	0.21588046131719
H	2.16643001082328	-8.12686379703268	-1.53325888055240
H	-0.18419772515797	-7.84347661455155	-0.74786526795663
H	0.22073612991856	-6.65098640211891	-2.03477763908341
H	-0.70703649613649	-3.94522957029937	-5.51293111891696
H	2.32630869019769	-6.91410631481907	-4.61154702766059
H	5.05748243610955	-8.91091179386966	0.83561476918882
H	3.92454365223926	-8.28731519112235	4.97642755623303
H	3.26981685828123	3.58957900213486	-0.83535762542415
H	5.80322955373629	0.44161872538187	0.67561539643917
H	4.51577205833788	-0.60633195335190	-0.04469476854207
H	4.67696589872220	-1.26270008557327	2.24367166899032
H	6.70894349376730	2.47759179811549	3.87750541578401
H	8.08607599623135	1.33307351691003	3.70511428737744
H	7.11463315136683	-0.05711802106990	5.66579862150563
H	6.22927022333592	2.87310999859492	6.25450258492465
H	6.41783546081868	1.46851674954711	7.48849675485603
H	0.28700884596567	-0.50135541879098	0.89745532865577

H	0.52060153240797	-0.03635942526602	2.60278748156363
H	0.14032768750059	-2.41512952884282	3.31120249432098
H	-3.11973105339242	-2.62063971050930	0.43421967521716
H	-1.59203650146753	-2.17068026040160	-0.36411592534166
H	-3.48952791804579	-1.42626781143337	-1.80268549248899
H	-4.16867432517423	0.92767878607917	-1.44924828631717
H	-3.37593538699438	0.89474257272465	0.26472658840228
H	2.22439872261825	3.49305109708805	1.41183292529321
H	2.45919496464394	5.20129730012467	0.92677558697888
H	3.57815853233130	4.45600177873575	2.11741019954699
H	5.62003694682811	4.44611642720936	-1.12193207046407
H	5.63335262495144	5.02655897659284	0.57822482159819
H	4.53140664304285	5.78289055295992	-0.62163707069857
H	-1.77652623810071	-1.04058994940153	3.26145801523487
H	-2.24784165684669	-2.62931982516646	2.55284251511226
H	4.58016985947938	1.72818475022441	3.04016899832218
H	4.52218228355862	0.32974971877540	4.17205246964170
H	-1.45596308873489	-4.77365323915193	0.63414559124053
H	-1.84186827726697	-6.53434004987982	0.35796908984964
H	-1.71426764666434	-5.39827508292857	-1.05241283812380

V-SR

92

Coordinates from ORCA-job 5-SR

C	3.93695056614557	-3.96740937219141	-4.71011359789713
C	3.06141833633797	-3.62834540895422	-3.66387038090811
C	3.50851109955795	-2.84944013988234	-2.54954523027446
C	4.86828120355488	-2.41106888376659	-2.58139100195381
C	5.74154758897403	-2.74180689046854	-3.62535460737955
C	5.26880267085722	-3.52649169099432	-4.68986399919313
C	1.64512691251229	-4.14581792859329	-3.63585144932803
N	0.54166975957627	-3.13995243881105	-3.64044957005202
C	0.44845723627537	-2.37896396088965	-4.89918572803296
C	1.46915628065018	-1.25688758962251	-5.03172664763739
O	1.44159585108840	-0.43565920327022	-3.85275831657467
C	2.23511392881242	0.75541770192500	-3.98237927452545
O	2.69282946604248	-2.54342596349033	-1.56434037010111
Y	0.88236200502011	-1.31829489251105	-1.64739822108368
O	1.38564724373339	0.61941547934599	-0.99310151370928
C	1.56039247557409	1.32447967989480	0.18298395003341
C	1.22483535269667	2.81321430909508	0.02825190342161
O	-0.14480337291799	2.98749042422883	-0.25684857807178
C	-0.52519901573497	4.33815920425550	-0.34928510724180
C	-1.95762641775017	4.48848082888852	-0.76923503693921
C	-2.78023680124334	3.47964202825543	-1.09824352417008
Cl	5.43645150888230	-1.40423272146401	-1.27049449389835
Cl	6.35137806032213	-3.95326956576938	-5.99874190182354
C	-0.72324454616455	-3.90204993927629	-3.38231205538744
C	-2.01728261076421	-3.12958188894663	-3.42907486781742

C	-2.21053650435614	-2.05971962743065	-2.49973685797453
C	-3.49628303519407	-1.43733867031168	-2.48999248789273
C	-4.52287240954174	-1.82687171345477	-3.35865064568307
C	-4.28958258758117	-2.86896147390729	-4.27065935797501
C	-3.04788742589214	-3.51913416706799	-4.30405697670494
O	-1.24421177782434	-1.67161584113387	-1.70116649145478
Cl	-5.56275288500025	-3.36080946146578	-5.36822765754084
Cl	-3.78277588171751	-0.15630189686292	-1.34052332555042
O	0.87575701982992	-1.60014332958094	0.68356649394428
C	1.04045558943369	-0.71864855250118	1.54621978874354
O	1.60735396232320	-0.99675285305352	2.71773927907565
C	2.18823891919420	-2.31904358382665	2.90096030121657
C	2.35683439856607	-2.46045777045424	4.41326294605210
O	2.79626746911787	-3.77699438981118	4.66448012719404
C	3.10250907435269	-4.03717404842503	6.02948591364694
C	1.88863706571956	-4.05649947139842	6.92120893656031
C	1.75592055745200	-3.34130107201016	8.05107310132548
C	0.69349410989463	0.72014028866482	1.34785574121766
C	3.49395025479362	-2.48913400702998	2.10872125552659
C	4.49899325964592	-1.37161513740086	2.33560087037786
O	5.61524233615578	-1.84078955185103	2.93842073295249
C	6.74696743947465	-0.94676006742815	3.19956834404843
C	7.34236318682829	-0.39130755118530	1.90763233415690
O	4.31662055473019	-0.20948671183033	2.00895282398990
C	6.39239764319300	0.11640555249501	4.23722109874544
H	1.50932172064747	-4.73166837183734	-2.70056366306852
H	1.49410298161932	-4.85402304296635	-4.48714525575350
H	-0.60278624764511	-4.35304752680705	-2.37163142086193
H	-0.79102538123174	-4.75279820221826	-4.10315512604416
H	-0.57009328317766	-1.94011793779332	-4.93728234411145
H	0.54437182382083	-3.04357134722015	-5.79472505374345
H	1.19791135742562	-0.63367276346809	-5.91430654594594
H	2.50198256649719	-1.63738319116441	-5.18293951703520
H	1.82278779138057	1.39926026677792	-4.78904885373110
H	3.28886817950881	0.49127612448788	-4.21823226921295
H	2.17900434566608	1.26751354676118	-3.00335934396011
H	6.78009019635051	-2.38518064638993	-3.60911198704037
H	3.58215949976413	-4.58260882695933	-5.55090219622233
H	-2.88834016189779	-4.34566081050534	-5.01284051127462
H	-5.49568954818756	-1.31868712356901	-3.32335135739281
H	7.47564145616087	-1.65282727564066	3.64931319405808
H	3.92735208570207	-3.46051435699234	2.41161452160641
H	3.27783485815644	-2.52220383145966	1.02024821765278
H	1.46179866466385	-3.07679049304426	2.54165081161106
H	3.85324158994539	-3.30356796872582	6.41517712505903
H	3.58396186536001	-5.03900406838744	6.02646700336882
H	1.07423283723371	-4.72861879190503	6.59313390193886
H	2.55324639546085	-2.66023120481635	8.39547892636690
H	0.85619831850954	-3.41475937571046	8.68196007138524

H	0.85869787233120	1.27595027192688	2.28948565101787
H	-0.36970360348190	0.80972613488651	1.04334789342708
H	2.62618428584552	1.28326485984037	0.52448041590402
H	0.12901025541351	4.88572579539289	-1.08032171286063
H	-0.36570312802732	4.86533316049777	0.63033374061543
H	-2.31545047664767	5.53371087807675	-0.79893517802983
H	-3.82102792168462	3.67173558587388	-1.40132451862934
H	-2.43922339065127	2.43338079225809	-1.07879615738163
H	7.50906070590428	-1.20407669050676	1.17330320884030
H	8.32170694733365	0.08041111825169	2.12635572286004
H	6.67810815850751	0.36567808590386	1.45066542645704
H	5.95738933490272	-0.35067026684355	5.14367669097282
H	5.66892404173837	0.84638540385109	3.82828501158850
H	7.31016169280301	0.65874934538404	4.54221748337624
H	3.09286619585955	-1.70618752369584	4.79030840876606
H	1.38235221715150	-2.23856157570252	4.90965824864332
H	1.50992433673366	3.35909569775557	0.96471264374399
H	1.85795344859850	3.22471007767764	-0.79749797441241

{ONOO^{Me2}}:

I-S

84

Coordinates from ORCA-job 1-S

C	-1.87662929995217	-4.10242065843377	-1.78927910139974
C	-1.00103400990148	-3.61013275399582	-0.80138179147955
C	-1.38970547072614	-2.50346737415925	0.00904028621467
C	-2.67410672905139	-1.91119963245956	-0.20112208473655
C	-3.51057247524190	-2.43656192045877	-1.19711268609122
C	-3.14188028884015	-3.53210684122632	-2.00994042590937
C	0.31886383655841	-4.27174266308183	-0.51045870118295
N	1.54087780442480	-3.44195344181796	-0.77936362510753
Y	1.38891571226132	-1.17024543663084	0.58746310677386
O	1.23053165304303	-0.43443950213591	2.84087243555672
C	1.17065025002215	0.72280018964339	3.28526310305780
O	0.65927282450277	1.00853960396452	4.47970125258170
C	0.07836310803036	-0.04749169286409	5.33628270549284
C	1.12864064427492	-1.06244692797757	5.77640687561613
O	-0.56569306912520	-2.03049325867175	0.94324892349563
C	-3.07993876492111	-0.74059416231999	0.65366386784838
C	-4.08118844749018	-4.06484359122812	-3.06612089597005
C	2.71810553781402	-4.22411443191740	-0.28510572981820
C	4.07739023346661	-3.57360523336960	-0.33839282610936
C	5.11857257305341	-4.13905729722300	-1.10100858462476
C	6.41652298405602	-3.59931427453500	-1.10806179091258
C	6.64804175292961	-2.46124581008512	-0.30334935146136
C	5.64707326564224	-1.86880277881476	0.48125598083492
C	4.32759569896836	-2.42260158899612	0.46679373764257
O	3.35608386084983	-1.86589104743241	1.18224432725007
C	5.91520871908846	-0.66845597392989	1.34869070461453
C	7.53088083794473	-4.21762241910015	-1.91893442725172
C	1.61695134573029	-3.11626011629718	-2.21585464203914
C	2.54988489781447	-1.95978578154020	-2.54545527053072
O	2.24465556247999	-0.85029107714277	-1.68695029363449
C	3.01997952350047	0.31893417990936	-1.99097800630286
O	1.05813540064660	0.91981026744762	0.37471298073511
C	0.88849715538016	2.04586616820592	1.14254324512077
C	1.62770892229197	1.93234942574037	2.52112837037912
C	1.35453318645775	3.31527618428261	0.41186780500650
O	2.74348717566631	3.24471738787241	0.15338188878809
C	3.23754826630480	4.35720793417575	-0.55146693238769
C	4.70550914916306	4.23135948504463	-0.83274431112675
C	5.48781342986402	3.21018355125895	-0.44679091849703
C	-1.17162150678734	-0.64751510643664	4.69920362762623
H	2.48124711530962	-4.46763853090844	0.77448134630074
H	2.75528356555376	-5.19466182538643	-0.83806155045618
H	0.36677020268053	-4.53189150305023	0.56893246913272

H	0.39663831377594	-5.22842249538050	-1.08206189006384
H	0.58770054778047	-2.85336807939010	-2.53834213771445
H	1.92941388418198	-4.00436297002890	-2.82085589472082
H	2.38728792986040	-1.65524566246587	-3.60539961137985
H	3.61893145416922	-2.23442518525318	-2.42160334405525
H	2.80296257202973	0.65811076224841	-3.02765039484263
H	4.10528952901134	0.09521096417648	-1.89740359960949
H	2.72362195618566	1.09834665582014	-1.26398799641995
H	7.65925055693565	-2.01849331182790	-0.28292755295588
H	4.90441993388700	-5.03716536458593	-1.70661601656593
H	-1.55921051058088	-4.96750272350496	-2.39748268406176
H	-4.49885196724191	-1.96857818226271	-1.34970541908984
H	-0.22275980391083	0.55546409934339	6.21713448764590
H	2.71047233957071	1.82615848616483	2.29874905985436
H	1.47708270128879	2.83895165959185	3.13727782573292
H	-0.19781751048984	2.23106817276678	1.37300591067759
H	3.05176861878728	5.30597440645561	0.02054415156451
H	2.68587625328517	4.49126217414762	-1.52024844471932
H	5.13383884065327	5.07514106838426	-1.40328434955307
H	5.07477049897925	2.36589187870047	0.12629310349626
H	6.56110628882597	3.19068056670804	-0.68969985054084
H	0.70694284967817	-1.68599763568174	6.59027121276877
H	2.02726892242527	-0.55086205592196	6.17469055110841
H	1.43270780537347	-1.72660323961418	4.94647269263729
H	-0.93647951148123	-1.25564483153125	3.80456347743450
H	-1.88379656741796	0.15036529152754	4.40868446949676
H	-1.67832436736930	-1.29622553567864	5.44183664006588
H	0.78138815603250	3.38862705047590	-0.54479047148814
H	1.11239255052268	4.22331093125246	1.02125143686561
H	6.97302381697249	-0.34679383785331	1.28576657552604
H	5.27179457875155	0.19189356557800	1.06281969351941
H	5.67340388964739	-0.88126181343800	2.41147474722866
H	8.03045671414564	-3.47108934818095	-2.57230286416138
H	8.32292183005540	-4.64934940179603	-1.26919678196503
H	7.15752166761922	-5.03393181424889	-2.56871764924280
H	-3.62877742972525	-4.90748171019053	-3.62567724657791
H	-5.03237141671966	-4.43237769446756	-2.62436543935488
H	-4.35743317624763	-3.28302306621573	-3.80581064107553
H	-4.10366830591477	-0.39500461747652	0.41078947437196
H	-3.04191886983975	-0.99886734642759	1.73332850307244
H	-2.38170269723036	0.11433446616253	0.52179517405209

II-SS

104

Coordinates from ORCA-job 2-SS

C	2.41185244090378	-3.20870921708302	-0.36613418429785
C	1.96893858053933	-4.22261780548980	-1.26847176641472
C	2.80675126007679	-5.31765668074939	-1.55556823417750

C	4.07886949886259	-5.46266770299998	-0.97427979384130
C	4.49654160944173	-4.45674889664328	-0.07593576640659
C	3.70098598519825	-3.34517831330694	0.23997661294914
C	0.57474960849336	-4.15965774521720	-1.84388608619641
N	0.21809053984439	-2.97135161155766	-2.67760011177481
C	1.16458186823556	-2.74739108605545	-3.78903146015152
C	2.29428792277775	-1.79586277273425	-3.40332636467469
O	1.77096254459987	-0.57119936220238	-2.86568696959331
C	1.55566874280093	0.47895009066268	-3.81108936660053
C	4.96706371549743	-6.64359537684376	-1.28802321074448
C	4.15897846305722	-2.27948570971475	1.19864702902525
O	1.66449038134686	-2.14455960597879	-0.11705700988752
Y	0.19000591391287	-0.80669104674808	-0.96646971560101
O	-0.43112148320413	-0.07109364247735	1.26304609117857
C	-0.31306325179312	1.04191460545972	1.80002535764524
O	-0.20984709247137	1.19926070140577	3.11876635665417
C	-0.13771067322529	0.03653926271040	4.02206643838367
C	-1.42524761432785	-0.78438108047693	3.99989536463344
C	-1.16475549107316	-3.19764964132794	-3.19459819875145
C	-1.74445888088634	-2.10796565507247	-4.06201029682046
C	-2.18209521170152	-2.39535783520635	-5.37059555583037
C	-2.81270545641259	-1.43463345298464	-6.18197447717384
C	-2.99732454944231	-0.14635121006439	-5.63092712464624
C	-2.57324299585923	0.19184343145971	-4.33685577604088
C	-1.92681228847214	-0.79680401911346	-3.52435041303626
O	-1.51663700642333	-0.48852636281542	-2.30589934930791
C	-2.77543256160534	1.56969416292120	-3.76494525132868
C	-3.25627802048753	-1.75121207714455	-7.59118307782998
O	-1.57351615580823	-2.35797432676705	0.05181498808429
C	-2.76355128292014	-2.13278881679958	0.14645145724801
O	-3.74178150500030	-3.05747399726488	0.33484905274922
C	-4.79126610736419	-2.00527526483770	0.20536226903473
C	-5.65376107252929	-2.25132090832637	-1.01517265270856
O	-4.83389404566924	-2.16259567531922	-2.15447538791008
C	-5.45047398262100	-2.51552169303066	-3.38209076091727
C	-5.56572312609254	-3.99880816499734	-3.62253488258952
C	-4.98069842157468	-4.95652367773037	-2.88284552690436
O	0.72905105538916	1.26841941152190	-0.90287771408193
C	0.76669086509299	2.37390704877039	-0.10120321080274
C	2.15777935427597	2.63908511090621	0.49486394351267
O	2.50745422829533	1.59680967163184	1.38960784863758
C	3.74453861798962	1.79873656790430	2.05539698888332
C	4.94383403621506	1.76375101337583	1.14307305337626
C	5.89884826333331	2.70805932888461	1.09939794521838
C	-3.68493181134873	-0.93688030086223	0.08377670806327
C	-0.32937736240875	2.32937619809057	1.02881916938074
C	1.13310401676206	-0.77464311997495	3.79261320608404
H	-0.16840413804162	-4.17917567459268	-1.01722886653612
H	0.40427173386045	-5.08403314029933	-2.45062134540549

H	-1.80828435846125	-3.34486952497753	-2.30206135284382
H	-1.19354610181472	-4.16183367413748	-3.76127172528131
H	0.59355407063921	-2.30454036436527	-4.63091751930397
H	1.60176650314580	-3.70618521373322	-4.16006982255901
H	2.93308448885581	-1.57485739546607	-4.28688226210384
H	2.93666435005990	-2.23371674081459	-2.61637630365759
H	0.78951055514346	0.20328757584672	-4.56908251120561
H	2.51029529469278	0.73336919276379	-4.32242664371450
H	1.20385623992098	1.34310385991273	-3.21705959114410
H	5.49048681934105	-4.54093062998934	0.39773577650241
H	2.44295063782090	-6.09130126663842	-2.25446594608052
H	-2.03238432453628	-3.41651129087315	-5.76285945055808
H	-3.48885589189496	0.63148309596108	-6.24164484431954
H	-0.06513347525699	0.54909541012533	5.00326711039770
H	-0.24436738665002	3.19080513782025	1.71797323410947
H	-1.31161028034151	2.38298080495682	0.51389629647926
H	0.52711023217558	3.31245721345793	-0.67555220840140
H	3.81779096316695	0.96578924563831	2.78924967450062
H	3.73495170375147	2.75814149641859	2.63263871315999
H	5.01667845315049	0.87188824390342	0.49409591277154
H	5.84402089787662	3.60935882645757	1.73439073730361
H	6.77530639975757	2.61641139216975	0.43869315104171
H	2.02359093235297	-0.11788586289628	3.82385435966819
H	1.11935525447661	-1.30005475913990	2.81870045089658
H	1.23279567780403	-1.52703955376461	4.60084475372402
H	-1.50670113470390	-1.38528923854836	3.07513613243439
H	-2.31297353853328	-0.12634929507453	4.09172493233180
H	-1.42839192719725	-1.47568488509608	4.86661748230285
H	2.88730071614407	2.70767108173763	-0.34555410002783
H	2.16485689506214	3.62537341130126	1.02737271757431
H	-3.57387119870844	-0.24713883773867	0.94190873093634
H	-3.60423709452317	-0.39577911779411	-0.87836983791827
H	-5.40141238284376	-1.98090020572561	1.13021305790810
H	-6.14299458953638	-3.25015440976073	-0.92274147313650
H	-6.46967720936092	-1.48307021242920	-1.03057259219308
H	-6.45809776853832	-2.03616172256733	-3.46734840264633
H	-4.81705710301232	-2.06174134754198	-4.17751895824055
H	-6.16921017069648	-4.27688096532159	-4.50634926588604
H	-5.09427678220618	-6.02170742913180	-3.13580075964994
H	-4.36392113784557	-4.70406715640368	-2.00507961418343
H	5.21654164151271	-2.42217264928659	1.49576317025656
H	4.03807707127994	-1.26949679620927	0.75431213327987
H	3.53834016866407	-2.27191605747969	2.12118620316764
H	4.48840244488309	-7.33111846568718	-2.01353422124541
H	5.20518795430362	-7.23546061639499	-0.37788557980545
H	5.94012813101241	-6.32698835283452	-1.72199829711357
H	-3.17683355003196	-2.83497994096099	-7.80885429309126
H	-4.30967407923993	-1.44924997548595	-7.77279070703201
H	-2.64104969961277	-1.21802086522707	-8.34886992352224

H	-3.24020531330664	2.25391009958838	-4.50173536438850
H	-3.42354255174420	1.54308291282141	-2.86174005129194
H	-1.81333210443585	2.00933288372021	-3.42646007995898

II-SR

104

Coordinates from ORCA-job 2-SR

C	-1.88556959950302	-0.73330095439596	-2.17488728140182
C	-0.93177835751468	-1.60079852529969	-1.60345093492978
C	-1.02623427347486	-1.94686538714207	-0.21969695704460
C	-2.09892729845495	-1.38989801029718	0.55188803626940
C	-3.02314971276239	-0.53516920784968	-0.06656987108408
C	-2.94664435065470	-0.18724741232150	-1.43312589500618
C	0.15497725353614	-2.19856458680850	-2.46458661450177
N	1.56106976661173	-1.92180146525387	-2.04586155209997
Y	1.99943157380156	-3.19773793587080	0.33840137477778
O	2.40168027964625	-2.84313719640372	2.40798783548150
C	3.03978636994108	-3.43428857366885	3.47216088078810
C	4.56500941632724	-3.26480546810806	3.34622256782053
O	5.20945021685564	-3.82524466165691	4.48046847685690
C	6.62553609000004	-3.81671440998618	4.40503226234594
C	7.22659148711518	-2.43740087864352	4.50146452236184
C	8.10484511682260	-1.91796793488405	3.62684665653976
O	-0.14639486299107	-2.75462675325203	0.35281206552528
C	-2.19527374925891	-1.73991518557374	2.01307086277970
C	-3.96945982502870	0.72896445476424	-2.06241288491763
C	2.45967114807191	-2.59049839733466	-3.03564331915134
C	3.94483203787613	-2.37751351206763	-2.87900349504281
C	4.69355509908943	-1.79039258340641	-3.91673483788661
C	6.08807681552695	-1.62989114185423	-3.83583192869898
C	6.72090463719560	-2.07694359514151	-2.65584828726346
C	6.01902758131475	-2.66307783380478	-1.59116602404903
C	4.60073682308910	-2.82587085086928	-1.69223244542270
O	3.90665496301846	-3.34430557689559	-0.68990889880087
C	6.71417686532525	-3.10565741223309	-0.33123682021958
C	6.88541938527879	-1.02547959399691	-4.96743844762168
C	1.80339777385247	-0.46853434987215	-1.93423044628778
C	2.81362695248277	-0.13236837917048	-0.83928999084250
O	2.44805532274532	-0.75449253484924	0.40136771580786
C	1.69299182838782	0.05031194625671	1.30888253223214
O	1.09467563960837	-5.13206540203972	-1.11599085251711
C	0.04661772541397	-5.73491659216382	-1.00898397074889
C	-1.42766496606651	-5.41814903832096	-0.86795877520896
C	-1.57408285603406	-6.95171762281688	-0.82872591062305
C	-2.05626850976626	-7.58791327880189	0.45796546706181
O	-1.58996853862001	-6.84776476000140	1.55667929540322
C	-1.95375821545465	-7.38839615094300	2.80936887534307
C	-1.63161489073331	-6.44366387026978	3.92880397344790

C	-1.12868314677022	-5.20564495320188	3.78744258614127
O	2.41641826528665	-5.38956756599469	1.27368660994486
C	2.88174968681011	-5.71778906610479	2.37652464247530
O	3.64361735522339	-6.80460213652993	2.51600830107338
C	3.92301173067684	-7.61302401262098	1.31855993940572
C	4.20261029958638	-9.01858077621808	1.82864218767380
O	-0.10055913794020	-7.08659585035297	-0.99501685670475
C	2.66148777666215	-4.94547808558020	3.64034145783457
C	5.07629304185733	-6.99001250417785	0.54065769964940
H	2.23110927176848	-3.67704709662145	-2.96510257767717
H	2.16347384414349	-2.26572207198029	-4.06446271797084
H	0.06662577936036	-3.30501665738116	-2.48951760697086
H	0.00785442385022	-1.84968969962721	-3.51752141473221
H	0.83427693508320	0.01206594610244	-1.68873639163865
H	2.14987990330948	-0.03150077957069	-2.90203393799888
H	2.88087179759058	0.96936085542165	-0.70272084141733
H	3.82281980137922	-0.50732632507651	-1.09430158987217
H	0.69437759864810	0.31455798387876	0.89559525975681
H	2.25318586977413	0.97973757863389	1.55301384744045
H	1.57420754867521	-0.56237835539442	2.22238782087283
H	7.81420776487047	-1.95723938867276	-2.55781099202108
H	4.16382274602793	-1.45310970731791	-4.82496330739552
H	-1.79046225530236	-0.47907659454772	-3.24527197939027
H	-3.83927425152755	-0.11513877745855	0.54728526695532
H	3.00471004129700	-7.59271405863333	0.69523355731820
H	3.23183539279699	-5.39920779973903	4.47147390262856
H	1.57567344044364	-4.99615024032166	3.86700424791222
H	2.74754004124769	-2.96129441248389	4.44683339710062
H	6.98218940637488	-4.32141882525832	3.47165904706018
H	6.96760483812038	-4.43066594195777	5.26770701311166
H	6.89768615771236	-1.84280248822819	5.37402847910664
H	8.43628510857600	-2.48740487511071	2.74130788471351
H	8.52996822864347	-0.91050486051928	3.75969212268896
H	-1.86929605307477	-4.88809878944503	-1.73310211300876
H	-1.66408856419486	-4.87415421405361	0.06499394566660
H	-2.07640242996143	-7.41444828660465	-1.70192393873837
H	-1.43972123994325	-8.37050673463611	2.97994346030655
H	-3.05168144891164	-7.61940250266093	2.83196817068866
H	-1.85672353560291	-6.84190076174692	4.93443675909438
H	-0.93899411761086	-4.57037533854449	4.66601883752982
H	-0.89494159143992	-4.78259367529226	2.79820311466239
H	4.81428255805021	-5.97556004651999	0.18087796151470
H	5.30897423655931	-7.61406490610517	-0.34565276688126
H	5.98794067428720	-6.93118530049388	1.17008286134512
H	3.34397366021093	-9.41026234368243	2.40867863661214
H	5.09910622184944	-9.03187127807294	2.48111200407737
H	4.38530622519147	-9.70057173346580	0.97475709916835
H	4.92059020388013	-3.75526586659117	2.40350825968884
H	4.78443747755743	-2.17631384801720	3.24033182194954

H	-1.69935011027016	-8.64803276364759	0.49055840475263
H	-3.17609230021984	-7.62385404893431	0.43276402925076
H	7.80950800770861	-2.95273191437896	-0.39801313142028
H	6.33805120773146	-2.55024752900082	0.55481681591950
H	6.52378385108939	-4.17872876786957	-0.11798000233406
H	-3.01974826423086	-1.19092548279388	2.50873713690993
H	-2.36709607277235	-2.82752722230107	2.16469403593961
H	-1.24668629685470	-1.51424192585607	2.54468686528196
H	-3.69998841318775	0.98384964582777	-3.10667495414427
H	-4.98062464632231	0.26704499351009	-2.08584433219851
H	-4.07121400668388	1.68213948149643	-1.50116659659567
H	7.59913496538201	-0.25592471577165	-4.60498296307124
H	7.48965075872726	-1.79067282642399	-5.50283281536394
H	6.22727557618435	-0.54510513202962	-5.71881362314851

II-SS-TS

104

Coordinates from ORCA-job 2-SS-ts

C	3.95295903270809	-7.51644418772531	-1.13148354028708
C	3.65544184539745	-6.18404821619646	-0.77940153829787
C	3.09014257144522	-5.89946483664784	0.49934690738632
C	2.84672246235721	-6.98302602437618	1.40304248185924
C	3.16379087607837	-8.29018029503148	1.00595127003989
C	3.71891567624348	-8.59180937238381	-0.25776322419904
C	3.98712820540859	-5.05195334304477	-1.71895650167259
N	2.84221945029064	-4.18368770513724	-2.14398357036658
Y	2.02550820231171	-2.80815522247131	0.00624779639138
O	2.33519799430601	-1.43170662918746	1.87817876446076
C	3.36806886010713	-1.37536465749704	2.81868582309559
C	3.79754741159737	0.08402839229192	3.03723152098921
O	4.78445636888858	0.12589873213421	4.05148235933306
C	5.32107531115753	1.41885865613791	4.29060233084211
C	4.34846046995647	2.35583966412535	4.95968592789789
C	4.02959849235905	3.58274251383066	4.51378581214236
O	2.78253550690329	-4.65873597238410	0.84912350260077
C	2.26004504370709	-6.67513592632151	2.75456144316608
C	4.05156824232036	-10.01461082951412	-0.64063818649892
C	3.38091600447266	-3.18591680001817	-3.11911347010749
C	2.40371025722341	-2.22717532035079	-3.75472914207945
C	2.28243385144870	-2.15481508198085	-5.15615280525303
C	1.44715319878060	-1.21592075227625	-5.78668742179079
C	0.72009595936481	-0.33488440458063	-4.95601706465257
C	0.80054599161806	-0.37151507588727	-3.55579190370520
C	1.65283345302020	-1.33564572232757	-2.93212495783432
O	1.71692200320735	-1.41950091377584	-1.61087641519270
C	0.00988088735701	0.56325718219270	-2.68048212487927
C	1.33066402755397	-1.13971490391785	-7.29086039478596
C	1.73348696672701	-4.98941569059985	-2.70164635822990

C	0.36457464520482	-4.38436501110102	-2.39574539525643
O	0.20811399109808	-4.14994338410999	-0.98522185083531
C	-0.37511778205783	-5.22471137797837	-0.24250163663248
O	0.24636136281639	-2.52748444711479	1.42808481255585
C	0.61021729099402	-1.81922895595291	2.40784957678671
C	0.04104589074144	-0.48825087272327	2.91474012580312
C	0.29564569551286	-1.09749565390681	4.30654164560860
C	-0.89809069361265	-1.33358474275717	5.21280678482513
O	-1.98257176229846	-1.80016454453149	4.45181542581406
C	-3.13660897393722	-2.09778396733056	5.19930635437705
C	-4.19930886189120	-2.70049654813231	4.32742226686961
C	-4.04478372317559	-3.00863264622179	3.02948561272534
O	4.36738075153955	-2.13989813614866	0.00998125050088
C	5.05296885410741	-1.95568579597282	1.02849818240827
O	6.27660393112982	-1.42931954986771	0.97710984667605
C	6.82424412087524	-1.04079358769073	-0.33109765393078
C	8.33494020378893	-1.15584134620453	-0.20027667849651
O	0.75961772494802	-2.35009011752021	3.69436166082748
C	4.57163553161382	-2.27595398309707	2.41249972158520
C	6.33156015820365	0.35773655366569	-0.68408064910859
H	4.15385139066769	-2.61182154695435	-2.56120630058936
H	3.91560994139104	-3.73627511255367	-3.93256396851259
H	4.72232202411849	-4.36480497860078	-1.24574533040057
H	4.48391600997413	-5.47318630122240	-2.62765444062165
H	1.79241219731411	-5.99842912143992	-2.24423044077637
H	1.83631840660135	-5.12326671955338	-3.80510629180816
H	-0.44438594987642	-5.05812102166397	-2.75445595032774
H	0.23779760185829	-3.40315575671544	-2.89025451500800
H	0.25612816861806	-6.13929330852426	-0.27603258247289
H	-1.38837064948886	-5.45334268967249	-0.63936600101287
H	-0.46129420943365	-4.87272007462693	0.80173035005172
H	0.05525631777617	0.41322700684441	-5.42227825967986
H	2.87146956138421	-2.85384756840789	-5.77548498132358
H	4.38995998569779	-7.71501882227525	-2.12583598339207
H	2.96805539856735	-9.11423946668521	1.71426250899979
H	6.43782901045669	-1.76939518032035	-1.07365143936772
H	5.38758516653119	-2.15112046754415	3.14714025245373
H	4.21605422090533	-3.32877485536651	2.39700310620048
H	3.01448505133278	-1.78207495510342	3.79724943027179
H	5.70326384224372	1.87548568399225	3.34336456751424
H	6.19542831783596	1.25130060341698	4.95713769559608
H	3.89136730617127	1.97006601762947	5.88996309471778
H	4.46772417061799	3.98721682713644	3.58504896479650
H	3.33050762507998	4.23559900887042	5.05989299860167
H	-1.03153931398352	-0.38536490096535	2.66687445906420
H	0.60631813770547	0.41861336363655	2.64078698192737
H	1.11413597040266	-0.62338082401359	4.89176641116680
H	-3.53838328390470	-1.17666861576936	5.70066975240417
H	-2.89643105517601	-2.80743345941335	6.03550898380136

H	-5.16012565278845	-2.89024921670101	4.83864252091326
H	-4.86925629197876	-3.45211091145807	2.45049756358319
H	-3.08811440728217	-2.82892806591387	2.51438886939133
H	5.22772910709749	0.38173464502650	-0.76860621621523
H	6.75281404868014	0.67002772048407	-1.66058056052376
H	6.65342175185031	1.09206451502524	0.08229675305448
H	8.63291726770682	-2.18505934898418	0.07973354365899
H	8.71962162828710	-0.45866151969603	0.57125981215915
H	8.81727725027123	-0.90563480034044	-1.16577820173861
H	-1.14366373091113	-0.37311523653149	5.73702311827550
H	-0.61121329002312	-2.07153996402202	6.00398485852082
H	4.18712340183076	0.51548493996631	2.07972736854688
H	2.89925260738989	0.68634730631687	3.31176127166750
H	2.09862936910859	-7.59600980364072	3.34823915003528
H	2.91998053993891	-5.99650406498982	3.33639854646791
H	1.29263092632903	-6.13708478262460	2.66492664926176
H	4.42377356965171	-10.07949971354025	-1.68236645764627
H	4.83517293619292	-10.44699934437598	0.01860841590546
H	3.16724405381584	-10.68232845954427	-0.55965707083381
H	1.92945676488025	-1.92977910568057	-7.78611741066217
H	0.27916555583771	-1.25566536664888	-7.63074788555791
H	1.68335826357641	-0.16151645096392	-7.68365030888555
H	-0.60388468974505	1.26292217891909	-3.28079845372822
H	-0.66255977029267	0.00152789140350	-1.99734635619329
H	0.67750544926919	1.15691605199751	-2.02040531520614

II-SR-TS

104

Coordinates from ORCA-job 2-SS-ts

C	3.95295903270809	-7.51644418772531	-1.13148354028708
C	3.65544184539745	-6.18404821619646	-0.77940153829787
C	3.09014257144522	-5.89946483664784	0.49934690738632
C	2.84672246235721	-6.98302602437618	1.40304248185924
C	3.16379087607837	-8.29018029503148	1.00595127003989
C	3.71891567624348	-8.59180937238381	-0.25776322419904
C	3.98712820540859	-5.05195334304477	-1.71895650167259
N	2.84221945029064	-4.18368770513724	-2.14398357036658
Y	2.02550820231171	-2.80815522247131	0.00624779639138
O	2.33519799430601	-1.43170662918746	1.87817876446076
C	3.36806886010713	-1.37536465749704	2.81868582309559
C	3.79754741159737	0.08402839229192	3.03723152098921
O	4.78445636888858	0.12589873213421	4.05148235933306
C	5.32107531115753	1.41885865613791	4.29060233084211
C	4.34846046995647	2.35583966412535	4.95968592789789
C	4.02959849235905	3.58274251383066	4.51378581214236
O	2.78253550690329	-4.65873597238410	0.84912350260077
C	2.26004504370709	-6.67513592632151	2.75456144316608
C	4.05156824232036	-10.01461082951412	-0.64063818649892

C	3.38091600447266	-3.18591680001817	-3.11911347010749
C	2.40371025722341	-2.22717532035079	-3.75472914207945
C	2.28243385144870	-2.15481508198085	-5.15615280525303
C	1.44715319878060	-1.21592075227625	-5.78668742179079
C	0.72009595936481	-0.33488440458063	-4.95601706465257
C	0.80054599161806	-0.37151507588727	-3.55579190370520
C	1.65283345302020	-1.33564572232757	-2.93212495783432
O	1.71692200320735	-1.41950091377584	-1.61087641519270
C	0.00988088735701	0.56325718219270	-2.68048212487927
C	1.33066402755397	-1.13971490391785	-7.29086039478596
C	1.73348696672701	-4.98941569059985	-2.70164635822990
C	0.36457464520482	-4.38436501110102	-2.39574539525643
O	0.20811399109808	-4.14994338410999	-0.98522185083531
C	-0.37511778205783	-5.22471137797837	-0.24250163663248
O	0.24636136281639	-2.52748444711479	1.42808481255585
C	0.61021729099402	-1.81922895595291	2.40784957678671
C	0.04104589074144	-0.48825087272327	2.91474012580312
C	0.29564569551286	-1.09749565390681	4.30654164560860
C	-0.89809069361265	-1.33358474275717	5.21280678482513
O	-1.98257176229846	-1.80016454453149	4.45181542581406
C	-3.13660897393722	-2.09778396733056	5.19930635437705
C	-4.19930886189120	-2.70049654813231	4.32742226686961
C	-4.04478372317559	-3.00863264622179	3.02948561272534
O	4.36738075153955	-2.13989813614866	0.00998125050088
C	5.05296885410741	-1.95568579597282	1.02849818240827
O	6.27660393112982	-1.42931954986771	0.97710984667605
C	6.82424412087524	-1.04079358769073	-0.33109765393078
C	8.33494020378893	-1.15584134620453	-0.20027667849651
O	0.75961772494802	-2.35009011752021	3.69436166082748
C	4.57163553161382	-2.27595398309707	2.41249972158520
C	6.33156015820365	0.35773655366569	-0.68408064910859
H	4.15385139066769	-2.61182154695435	-2.56120630058936
H	3.91560994139104	-3.73627511255367	-3.93256396851259
H	4.72232202411849	-4.36480497860078	-1.24574533040057
H	4.48391600997413	-5.47318630122240	-2.62765444062165
H	1.79241219731411	-5.99842912143992	-2.24423044077637
H	1.83631840660135	-5.12326671955338	-3.80510629180816
H	-0.44438594987642	-5.05812102166397	-2.75445595032774
H	0.23779760185829	-3.40315575671544	-2.89025451500800
H	0.25612816861806	-6.13929330852426	-0.27603258247289
H	-1.38837064948886	-5.45334268967249	-0.63936600101287
H	-0.46129420943365	-4.87272007462693	0.80173035005172
H	0.05525631777617	0.41322700684441	-5.42227825967986
H	2.87146956138421	-2.85384756840789	-5.77548498132358
H	4.38995998569779	-7.71501882227525	-2.12583598339207
H	2.96805539856735	-9.11423946668521	1.71426250899979
H	6.43782901045669	-1.76939518032035	-1.07365143936772
H	5.38758516653119	-2.15112046754415	3.14714025245373
H	4.21605422090533	-3.32877485536651	2.39700310620048

H	3.01448505133278	-1.78207495510342	3.79724943027179
H	5.70326384224372	1.87548568399225	3.34336456751424
H	6.19542831783596	1.25130060341698	4.95713769559608
H	3.89136730617127	1.97006601762947	5.88996309471778
H	4.46772417061799	3.98721682713644	3.58504896479650
H	3.33050762507998	4.23559900887042	5.05989299860167
H	-1.03153931398352	-0.38536490096535	2.66687445906420
H	0.60631813770547	0.41861336363655	2.64078698192737
H	1.11413597040266	-0.62338082401359	4.89176641116680
H	-3.53838328390470	-1.17666861576936	5.70066975240417
H	-2.89643105517601	-2.80743345941335	6.03550898380136
H	-5.16012565278845	-2.89024921670101	4.83864252091326
H	-4.86925629197876	-3.45211091145807	2.45049756358319
H	-3.08811440728217	-2.82892806591387	2.51438886939133
H	5.22772910709749	0.38173464502650	-0.76860621621523
H	6.75281404868014	0.67002772048407	-1.66058056052376
H	6.65342175185031	1.09206451502524	0.08229675305448
H	8.63291726770682	-2.18505934898418	0.07973354365899
H	8.71962162828710	-0.45866151969603	0.57125981215915
H	8.81727725027123	-0.90563480034044	-1.16577820173861
H	-1.14366373091113	-0.37311523653149	5.73702311827550
H	-0.61121329002312	-2.07153996402202	6.00398485852082
H	4.18712340183076	0.51548493996631	2.07972736854688
H	2.89925260738989	0.68634730631687	3.31176127166750
H	2.09862936910859	-7.59600980364072	3.34823915003528
H	2.91998053993891	-5.99650406498982	3.33639854646791
H	1.29263092632903	-6.13708478262460	2.66492664926176
H	4.42377356965171	-10.07949971354025	-1.68236645764627
H	4.83517293619292	-10.44699934437598	0.01860841590546
H	3.16724405381584	-10.68232845954427	-0.55965707083381
H	1.92945676488025	-1.92977910568057	-7.78611741066217
H	0.27916555583771	-1.25566536664888	-7.63074788555791
H	1.68335826357641	-0.16151645096392	-7.68365030888555
H	-0.60388468974505	1.26292217891909	-3.28079845372822
H	-0.66255977029267	0.00152789140350	-1.99734635619329
H	0.67750544926919	1.15691605199751	-2.02040531520614

III-SS

104

Coordinates from ORCA-job 3-SS

C	1.57298703665104	-1.55215899869068	-2.97597021786724
C	2.29930105442993	-2.48288371093488	-3.77742081451453
C	2.03654280196011	-2.57780264485269	-5.15772711977168
C	1.07158031068733	-1.77405384729733	-5.79016998921359
C	0.36712570860364	-0.85256934649392	-4.98338592966035
C	0.59375146232410	-0.72004614328944	-3.60500953529016
C	3.38629285522873	-3.31141437294732	-3.14104834135323
N	2.99299337181049	-4.26269463985590	-2.05503192757036

C	1.98905232743826	-5.25664128281056	-2.48402851110385
C	0.55266069361951	-4.75651960443217	-2.44269389879474
O	0.28174659052892	-4.18119412551617	-1.15549680784837
C	-1.09951916822555	-3.84204209507190	-0.99317103062217
C	0.80559414963240	-1.87009800939891	-7.27405155028727
C	-0.16714342589901	0.26402971338558	-2.75749999756118
O	1.78045849367762	-1.47952988684295	-1.66965627001926
Y	2.06670723236787	-2.86171385298412	-0.02587029824895
O	4.33126234135377	-1.98204657625608	0.10336862537038
C	4.97897313866078	-1.71403916628668	1.12621678824214
C	4.45577035283840	-1.92842061742042	2.52044472578883
C	3.20575403841084	-1.06581449924600	2.81425407868016
C	3.51656554002640	0.43638066400029	2.81429384201525
O	4.51731933228329	0.68409483158779	3.78254972699073
C	4.95020942321129	2.03696897610163	3.84000026467961
C	3.91195227288502	2.97404312831843	4.40062350715705
C	3.49044278977500	4.10117730965210	3.80262972832662
C	4.25055139427794	-4.94451110769356	-1.59746061031218
C	4.09562776296984	-6.04787425661883	-0.58104836796299
C	4.61494490964227	-7.33302117213675	-0.83913855333457
C	4.55219173780673	-8.36762382168168	0.10900404335449
C	3.93599213513540	-8.07640267906060	1.34694894714206
C	3.39849059092026	-6.81746241240215	1.64950825813737
C	3.47450579376583	-5.77455888370469	0.67308770405558
O	2.96123406004318	-4.57999254081951	0.93052766642343
C	2.73620156765888	-6.52084916740543	2.96780407293401
C	5.11876533459139	-9.73930887858785	-0.17220306600692
O	2.18566228285375	-1.33685573913416	1.86518331811474
C	0.72692786222170	-1.73361258500301	2.30787971853984
O	0.81530448059447	-2.31129685184215	3.62586663923716
C	0.10755922807473	-1.18522043775614	4.22145297629814
C	-1.13314281310485	-1.62204009171570	4.98125618008859
O	-2.06889917569555	-2.17901985423628	4.09397946968524
C	-3.24749810614465	-2.64254446426568	4.70342435075208
C	-4.10981759228808	-3.36993871189954	3.71301155778450
C	-3.74789762932818	-3.65198695148072	2.45087607583972
O	0.31806828332893	-2.48141809874969	1.33105439811995
C	-0.07546468801504	-0.52289527590258	2.84492059552681
O	6.20526565195395	-1.19738609651529	1.07927748652789
C	6.81559526465140	-0.94147789720305	-0.23515422453878
C	6.34245096403029	0.41182757867322	-0.75245115364378
C	8.31770712811509	-1.03824606412025	-0.02037620493712
H	4.14144338920807	-2.63539855568636	-2.68067513283924
H	3.91433109734600	-3.88689125376566	-3.94114144055793
H	4.89436441138143	-4.13358829249783	-1.19053233846930
H	4.78226083794399	-5.35480344155406	-2.49062122200218
H	2.08345018744039	-6.12327890916197	-1.79841746357775
H	2.19968519083223	-5.63272378947082	-3.51565250735575
H	-0.12852910528664	-5.62463795820683	-2.60283296934945

H	0.34366614026429	-4.00341468092446	-3.23248674925993
H	-1.72650254917766	-4.75902488515690	-1.05341014604920
H	-1.41945671398029	-3.12813269170089	-1.78464220454716
H	-1.20134576832904	-3.37232407184857	0.00136389610147
H	-0.39621575663056	-0.20704041669692	-5.45227628438514
H	2.61171823457536	-3.30408776519424	-5.75851384848777
H	5.08987894031234	-7.52577719735128	-1.81710689562504
H	3.86726578289636	-8.87157229164705	2.10982170260749
H	6.46342700690603	-1.74386657714059	-0.91614845639429
H	5.24049180754737	-1.69530283979257	3.26226825545458
H	4.16044430143684	-2.99780629349361	2.59389649207052
H	2.85005151624442	-1.36678838328571	3.82320441850949
H	5.28489137087269	2.39219034935588	2.83335063953389
H	5.84181790408066	2.02597274728228	4.50421785319274
H	3.49778295166285	2.68081708987207	5.38314564259364
H	3.88448905149197	4.41105663904471	2.81937993243900
H	2.74674446633369	4.76395848801884	4.27239463712505
H	-1.11701100104119	-0.53811541734270	2.47735349089271
H	0.38135145833306	0.47234673381354	2.69954685144810
H	0.76791532782667	-0.62705271785695	4.92626706058450
H	-3.82676204749117	-1.79417212819538	5.15802697328503
H	-3.01047826712009	-3.32873169324368	5.56015795312701
H	-5.09744362061029	-3.68021058794292	4.09874543181881
H	-4.42483561660968	-4.19480931914411	1.77344189599430
H	-2.75803176629096	-3.35084018328973	2.07295491827399
H	5.24493245668303	0.42092816652240	-0.89917471115045
H	6.81627658866987	0.62654786588845	-1.73114663348920
H	6.62271928721551	1.22126414117323	-0.04785121837746
H	8.59925958346088	-2.03202983941796	0.37897581587216
H	8.66654057465211	-0.26321178860129	0.69156519343447
H	8.84597226029320	-0.88873590037642	-0.98262409835022
H	-1.55582698161060	-0.73217431457453	5.51776246103131
H	-0.83170561116588	-2.36170246419587	5.76568462256876
H	3.85270584223175	0.75768707561352	1.79504945263501
H	2.58197171021607	1.00487492435286	3.03152168001154
H	-0.88279540336883	0.85536429641862	-3.36157556188793
H	-0.73011409303638	-0.24789636312032	-1.94741621650300
H	0.52188361162249	0.96565270299427	-2.24109182740143
H	1.35639008584592	-2.71526672203328	-7.73279572368578
H	-0.27371260118930	-2.01608356379076	-7.49226558985621
H	1.11397571657310	-0.94601168293353	-7.81001148908522
H	5.53189522738770	-9.80697335786043	-1.19825515151546
H	5.93723533792051	-10.00056612302970	0.53298449450727
H	4.34847764517091	-10.53357362955937	-0.06974515789893
H	2.71559990561477	-7.41324215629102	3.62332950140601
H	3.25889037029945	-5.70317466635395	3.50932919982480
H	1.69598817180472	-6.15994404777608	2.82377524640861

III-SR

Coordinates from ORCA-job 3-SR

C	4.48102481004454	-0.78938197949015	-0.62554580668723
C	4.57731505118828	-0.90453560802302	-2.04405234162145
C	5.44999970775134	-0.06013230624101	-2.75766625831322
C	6.25061450074675	0.90027365246737	-2.11472733009966
C	6.14877470505966	0.99284964805628	-0.70885860282009
C	5.29082704732758	0.17902368119323	0.04613695197399
C	3.80077981720430	-1.98526258942873	-2.75460832898709
N	2.31007641383146	-1.95914837002412	-2.64623810558489
C	1.72278209335298	-0.66778296893365	-3.06408955320690
C	1.54623880724709	0.29569580787417	-1.89130508183733
O	0.81041153242967	-0.32312550085002	-0.82099302634434
C	-0.60648066634498	-0.11974995557463	-0.83491865239417
C	7.19224297280111	1.79509978294978	-2.88580361927217
C	5.18055549725960	0.29695911018808	1.54243732227999
O	3.63078965358453	-1.54387713722803	0.05560047029648
Y	1.69333629144976	-2.48220543752603	-0.08287222425925
O	2.81795107993887	-4.61289382444296	-0.41607237157865
C	2.63569442255884	-5.72984012570921	0.08898887905153
C	1.62799426469598	-6.01344890304225	1.17407625622894
C	1.77887941597109	-5.07934345367782	2.39297317811862
C	3.15017439406779	-5.18798408881394	3.06877997136839
O	3.39066475717165	-6.54360096493216	3.39622893201644
C	4.66883948068946	-6.78610823551203	3.97642042979600
C	4.82438212292863	-6.20603444360211	5.35810407164679
C	5.82411645827799	-5.39138243164401	5.73597868744856
C	1.78714898491895	-3.09462413719035	-3.47342563388327
C	0.28846386358592	-3.22070091860070	-3.56858261633690
C	-0.36148858544175	-3.18296890723493	-4.81894601042285
C	-1.74949191987768	-3.36356050930892	-4.94411546273916
C	-2.48373868899799	-3.58740798321885	-3.75746462803999
C	-1.88485039550525	-3.63226581345688	-2.49013003288428
C	-0.47010322057627	-3.44153599134517	-2.38078895892847
O	0.11735027791595	-3.45941868257036	-1.19481409319293
C	-2.67529187520266	-3.87983156498256	-1.23365165243466
C	-2.43784265649569	-3.32907475678057	-6.28829389842350
O	1.61490122188885	-3.72094883535325	1.99510652648844
C	0.48718706116359	-2.86211339535060	2.50983891936273
O	-0.72532436697257	-3.68416927806404	2.56020590653775
C	-0.99212790140048	-3.23657639873677	3.91390081446449
C	-1.48980424428964	-4.32090938843306	4.84698314298598
O	-0.52390363101689	-5.32102641622489	5.10956007716462
C	-1.00367772896866	-6.25430661849083	6.05319032460723
C	-0.05711848294096	-7.38337297885130	6.32244980972172
C	1.11529330699217	-7.62270873669202	5.71383551994544
O	0.47497730011321	-1.84212567420624	1.69346825239623
C	0.42446152494286	-2.65317313538375	4.04580128646090

O	3.32783796288122	-6.80304810634005	-0.28699751104420
C	4.33789974429711	-6.66031842131740	-1.34713385711670
C	5.64896242224091	-6.19299229559211	-0.72608499463995
C	4.41853917243215	-8.01669011387979	-2.02959537947602
H	4.10935012044532	-2.98058492834158	-2.36152600842622
H	4.08023008376262	-1.96966998431313	-3.83737083846958
H	2.21605378144377	-4.01567552754706	-3.01899331792185
H	2.21020590630053	-3.02117923333971	-4.50569996473726
H	0.72929561182423	-0.88351706318494	-3.50811161559022
H	2.33477086911411	-0.17151534291993	-3.85524613002328
H	1.01866172387484	1.21657301292611	-2.22329870058331
H	2.52266465684825	0.59448327500177	-1.46539884215711
H	-1.07555182302362	-0.55270563123677	-1.74517286084421
H	-0.83357824249747	0.96697948633630	-0.77536211831877
H	-0.99851560879737	-0.62941659610059	0.06467863401294
H	6.76466724119371	1.73872541839055	-0.17649148497623
H	5.51025218676251	-0.16554397833856	-3.85512409612160
H	0.24457215128133	-3.01196675377387	-5.72598750566559
H	-3.57620133683548	-3.73286881093032	-3.82512771409737
H	3.96147609974204	-5.88863545963322	-2.05044524492176
H	1.71542656811971	-7.06675164012897	1.49556486773908
H	0.61838820313926	-5.84507481274016	0.74135668117050
H	0.97374136313980	-5.34542241997084	3.11039997650078
H	5.48174840125604	-6.40873753696963	3.30741154472541
H	4.75591803850786	-7.89353337253460	4.01973649771890
H	4.04624372111031	-6.50148719142940	6.08605534774033
H	6.60771358627199	-5.07574628577472	5.02566324559651
H	5.90606585595288	-5.01506798851180	6.76778804374950
H	0.52716825924847	-1.60178954136037	4.37005164202437
H	1.09933284075275	-3.31442649321268	4.62103474807053
H	-1.77716490621884	-2.44307105720529	3.90574453983511
H	-1.98385315185633	-6.68451178831112	5.71331780571571
H	-1.23930516651238	-5.73881898030999	7.02277859558289
H	-0.41500685077022	-8.07161934000244	7.11013851122541
H	1.71781519058233	-8.50068406547028	5.99611650205181
H	1.51832269791826	-6.97921143260096	4.91839416472304
H	5.53487370424394	-5.19838945619361	-0.25273671656792
H	6.42738183510937	-6.10738484975762	-1.51042938234614
H	6.00273741459606	-6.91839832801349	0.03459131820316
H	3.43371585205934	-8.31501728983447	-2.43881680885677
H	4.75397126086992	-8.79846228103719	-1.31863612868502
H	5.14317488652458	-7.97427547257909	-2.86653097591769
H	3.94013529465109	-4.79777155936473	2.37777169678673
H	3.16384203097379	-4.53098515269187	3.96960383204073
H	-2.40997294687130	-4.77483127801334	4.39949399225027
H	-1.80816485046106	-3.82894408571481	5.80192003553752
H	7.10007849502960	1.63778426729589	-3.97886963900592
H	8.25397211562281	1.61027475958374	-2.61319823171579
H	6.99766599104985	2.87045816036721	-2.68553793072456

H	5.85900204262943	1.07626685957201	1.94122640872645
H	4.14172543001388	0.54180207639210	1.85085933069084
H	5.41962365997916	-0.66664472804320	2.04073247761656
H	-3.75946270894221	-3.96447797569943	-1.44366377027121
H	-2.34342079606028	-4.81087433732546	-0.72598864526002
H	-2.51606240080074	-3.07314876864574	-0.48748541111165
H	-1.72487455705182	-3.09962300248178	-7.10501716135104
H	-2.91856101313911	-4.30136166624256	-6.53140745495055
H	-3.24162858902789	-2.56262012846194	-6.32202843820843

III-SS-TS

104

Coordinates from ORCA-job 3-SS-ts

C	3.23835504034949	-5.38253848020974	1.56733530091033
C	3.88769171765988	-5.79795592282390	0.36582645050538
C	4.68227451793621	-6.96038363760848	0.35183018210155
C	4.90082854556210	-7.73132566839672	1.50574481818909
C	4.30095354451790	-7.27880007997353	2.69993715878055
C	3.48861250919379	-6.13596008612048	2.76148232561967
C	3.82883408477990	-4.92283847381743	-0.85703109718524
N	2.48771080196130	-4.53345448354942	-1.38679060983386
Y	1.28481369514300	-2.83977862790749	0.45398848905821
O	-0.30492625706275	-1.12798387040285	0.68717272943967
C	-0.17970434697147	-0.69388671142679	1.88057936686285
C	-1.09313608552465	-1.18528756176375	3.01946137137614
C	0.00128090453454	-2.12531060971304	3.55815208798132
C	-0.29287586947766	-3.61284034695592	3.53960021091025
O	-0.54482702393634	-4.03385711606851	2.18988547235173
C	-0.84867758104072	-5.42382005026716	2.11062076225140
C	-2.28784408117960	-5.77065163005648	2.38859047188714
C	-3.30298569248279	-4.89826030471939	2.50801499653873
C	5.74212521201979	-8.98524376524143	1.47929956373394
C	2.89401238475581	-5.68106007108790	4.06757632766064
O	2.43963652857638	-4.32760810040059	1.57356434619878
C	2.75132179682167	-3.87371266751149	-2.69957604400608
C	1.58810230066659	-3.23994704254440	-3.40826425218529
C	0.90775589179600	-2.18152843792429	-2.73840436294611
C	-0.18511262158344	-1.54159366914987	-3.41406294974453
C	-0.53122661387420	-1.97058691265839	-4.70647143052015
C	0.15071424856561	-3.00475837360934	-5.38681221139442
C	1.21420015060633	-3.62677544808519	-4.70856982230199
O	1.27262576753976	-1.83030187997201	-1.51777278971874
C	-0.23836366149598	-3.40256549419671	-6.79120197900829
C	-0.93624672818382	-0.43433669284524	-2.72157940821325
C	1.59105975698168	-5.69447417267792	-1.48292400184435
C	0.12543903911379	-5.33380037510675	-1.70038390337107
O	-0.27875640808848	-4.32864340420760	-0.75603502150834
C	-1.61806496957305	-3.86322712349807	-0.96962112265966

O	1.03390722926134	-1.77792721913940	2.62850310778761
O	3.07387998463477	-1.32729530891235	0.67395291181737
C	3.52312972412698	-0.32752155930195	1.24748185614944
O	4.82367083462757	-0.03671835396801	1.23580136135057
C	5.74237937159069	-0.94246931725234	0.53477758459287
C	7.08720538625234	-0.78895544382723	1.22829743942100
C	2.72520647525030	0.64157091756825	2.07842206824605
C	1.38417365091999	1.18107910223871	1.49616836887962
O	0.23499532021311	0.59721850329400	2.12775869025646
C	1.34147729768588	1.23206042545232	-0.03806059806988
O	2.54292268764062	1.90489245723455	-0.41289628200165
C	2.77264455923918	1.94968711612050	-1.81648312092347
C	1.88591768779836	2.93296912813008	-2.53537026037171
C	1.23895192967519	2.68379174599756	-3.68699025863719
C	5.76164304397234	-0.58927183701125	-0.94796672165389
H	3.50562204233748	-3.08583086320060	-2.47852331447652
H	3.24497163632505	-4.61231471179149	-3.38008346331179
H	4.35424528857594	-3.96108598476062	-0.65338549105939
H	4.40815767305409	-5.42553015234308	-1.67099114047160
H	1.69858657200110	-6.26610102962402	-0.53772555678365
H	1.89201224856624	-6.39095691584312	-2.30766176844754
H	-0.49855162083056	-6.24710083690985	-1.55011654880866
H	-0.05823503840494	-4.95335216447645	-2.72625973844962
H	-2.34737362946940	-4.67802406676617	-0.76658990176180
H	-1.73440755444471	-3.49859265673482	-2.01275984962797
H	-1.78735823601791	-3.02582760506777	-0.26754227009744
H	-1.37965313909471	-1.47350142490007	-5.20936428894368
H	1.77096927082588	-4.44232950708347	-5.20335065766542
H	5.16195833348660	-7.26039938052207	-0.59640340064113
H	4.47930125583332	-7.84204211442401	3.63283914514899
H	5.34951825712221	-1.97197521797828	0.67086197142048
H	3.39186530172826	1.48801548411743	2.32049757652300
H	2.47605305231530	0.10644865609387	3.01888617005310
H	1.32973531275935	2.23198367916419	1.84536045098190
H	2.67461405122680	0.93388337822886	-2.26955653819605
H	3.83422901369590	2.26758739272647	-1.92205998549645
H	1.81074133371205	3.92861213671648	-2.05958835805013
H	1.29713354622154	1.69666375898463	-4.17663854455421
H	0.63475323581973	3.45570551524182	-4.18937377307232
H	-1.99543372111934	-1.68531350051111	2.61974813514644
H	-1.38164552946044	-0.37420055336387	3.71285931775583
H	0.30057214810443	-1.87112984818306	4.60331195287853
H	-0.17644235943601	-6.00020591516737	2.78968307291792
H	-0.58453678442745	-5.74230364636403	1.08029297712758
H	-2.48475767718408	-6.85525200917015	2.47692346476406
H	-4.33166493490462	-5.23980718613568	2.69854371424824
H	-3.13462410482879	-3.81308160465609	2.41847257939571
H	4.75853871253301	-0.71579232088943	-1.39956076360404
H	6.46757000215875	-1.25494260015371	-1.48407652932331

H	6.09221662130184	0.45870795201693	-1.09698564550791
H	7.00852760150483	-1.03451499355749	2.30529139150690
H	7.46708934826409	0.24819368833371	1.13131306384632
H	7.82736365693752	-1.47469684154516	0.77083710617107
H	-1.17249038631733	-3.83993680839662	4.18459337384294
H	0.58756363099453	-4.16863096310284	3.92754506257562
H	1.28906203580233	0.22548154580987	-0.50402324172851
H	0.43291407041331	1.79555601894115	-0.35485532911891
H	-1.89052084476361	-0.20893995416910	-3.23803607389487
H	-1.13972080038354	-0.68313527023530	-1.66056161366257
H	-0.34322296385762	0.50550794491019	-2.69655232370048
H	0.24891977766945	-4.35013591545450	-7.09649051286090
H	-1.33546202174525	-3.54023799214165	-6.89367415347555
H	0.05390755951706	-2.62983852414266	-7.53597745680434
H	6.27226601478429	-9.09944464529974	0.51281253689897
H	6.50779929065104	-8.98561149924123	2.28368989256287
H	5.12740785966691	-9.90013671009602	1.62724642529303
H	3.39581620528289	-6.16413423375466	4.92893363330993
H	2.96892705736299	-4.58011976429091	4.17946669396178
H	1.81170464663900	-5.92971728296245	4.13911795250640

III-SR-TS

104

Coordinates from ORCA-job 3-SR-ts

C	-1.34746865697066	-2.96118079127633	-2.03020261775370
C	-0.76620383854801	-3.19893009364052	-3.31105994452136
C	-1.56435944663180	-3.13594991043565	-4.47043344373765
C	-2.93855897126122	-2.84762254025243	-4.41543689044481
C	-3.50056846374596	-2.61901246076535	-3.13956726971625
C	-2.74814849322705	-2.66935753514600	-1.95690402728813
C	0.69072892371870	-3.56835299770388	-3.39881733966780
N	1.65970678876214	-2.58336565678916	-2.81542632582980
Y	1.40390681214371	-2.74997729712190	-0.16500909288596
O	0.43454804604025	-3.97246964823076	1.59849328256603
C	-0.67092241536272	-3.65049423929249	2.44290817235216
C	0.11579756248187	-2.90424572836689	3.53841636906356
C	1.33496668660264	-2.73521414640382	2.61817484937125
O	1.43511389641681	-1.69604408510345	1.88843999606525
C	-3.79014604420316	-2.78923957542507	-5.66154932710382
C	-3.37315054898446	-2.44590325198907	-0.60571475898107
O	-0.61081342508180	-3.01136338952845	-0.93396400710512
C	3.03290136319964	-3.05237983101991	-3.17364907721214
C	4.19247556073311	-2.17085023396835	-2.78293998289873
C	4.37355217356947	-1.82580251260887	-1.40997183874083
C	5.52136686104123	-1.05283170599805	-1.03980670208252
C	6.42682012747543	-0.65520621211327	-2.03501009799096
C	6.25729147281290	-0.98077108080956	-3.39972614136171
C	5.12548366843576	-1.73985071961147	-3.74592464411026

O	3.49019621812725	-2.19516262003049	-0.50138500100711
C	7.25856176458332	-0.52850576865733	-4.43649726170033
C	5.70113408045296	-0.68539569559449	0.40851615135651
C	1.38474190809002	-1.20031749456506	-3.26713926572677
C	1.68942932228067	-0.15116020401967	-2.19608654230090
O	1.01642840006544	-0.44729727665757	-0.95714854582430
C	-0.25113929579876	0.18675385877306	-0.78422156934818
O	2.62748044568362	-4.84457104503958	0.07257500031700
C	3.21140705156814	-5.37311938923980	1.02970487896524
O	4.51485679966578	-5.64917848187971	1.00715250769180
C	5.30690468346902	-5.21360032632670	-0.16020562777387
C	5.26544486649265	-6.30462893108405	-1.22234400059436
C	2.54724317425837	-5.76254708286653	2.32608374156293
C	2.62328649938645	-4.66528914527351	3.42589407915147
C	3.92243650596715	-4.71295398445785	4.23146167341580
O	3.99375643861003	-5.98182830207647	4.85464198243347
C	5.18720872757776	-6.20147427256707	5.59703198136192
C	5.26956207435769	-5.37614529803743	6.85470048573077
C	6.31159564884736	-4.59928387360875	7.19583836077624
O	2.54995851337934	-3.33664842294992	2.89576109314583
C	6.70102934360245	-4.91489790353719	0.36663977433741
C	-1.45674000484880	-4.88294206696258	2.86259502969472
O	-0.67292619628054	-5.75614764915883	3.65898556157690
C	-1.39028247868285	-6.90394274866320	4.05141305896669
C	-0.59536185100235	-7.83252237173729	4.91886778906449
C	0.66997956477143	-7.67283697144702	5.33945594867748
H	3.14266290717677	-4.05362322193689	-2.69673828516501
H	3.07459755900387	-3.22502432790950	-4.27756641089681
H	0.87574958263332	-4.53083268653959	-2.86619807075986
H	0.95179318812778	-3.75118156435568	-4.46981176195743
H	0.30931282068347	-1.14573256923630	-3.53266911990023
H	1.96160195967934	-0.94723952164483	-4.18826153095433
H	1.37899950363455	0.85473564114339	-2.55428933483112
H	2.76882775640505	-0.11244973101920	-1.96207431310756
H	-0.98738846359827	-0.14041489364709	-1.55007639171622
H	-0.13262068031895	1.29168860382575	-0.82255728897116
H	-0.62020701338973	-0.09867252800544	0.21820549338560
H	7.30419754215898	-0.05603002323056	-1.73431214571847
H	4.96288971104088	-2.01507189551546	-4.80283503864558
H	-1.09115127542636	-3.32388060715529	-5.45004070698917
H	-4.57876028871315	-2.39328244382488	-3.06418317937760
H	4.82929877093475	-4.28746839926366	-0.53621740228452
H	3.04206340951467	-6.66221504897052	2.74099811395500
H	1.48429737102630	-5.96550986779490	2.11473132486623
H	1.77582684235900	-4.85692756430840	4.11664433759827
H	6.08933766983549	-6.02556716618916	4.96049384942768
H	5.16623038527547	-7.28203541255765	5.85796848044120
H	4.39332609772941	-5.45225188179884	7.52488260805355
H	7.19396625189337	-4.50242007559706	6.54001698251781

H	6.33115949111831	-4.03834342058786	8.14351958182016
H	-0.28216535852886	-1.92179102093098	3.85671004551057
H	0.30182000614025	-3.53982312228987	4.42452375621536
H	-1.39768733659658	-2.97947709296187	1.92296575431550
H	-1.75140605749215	-7.46901078624797	3.15106202841975
H	-2.32588394833443	-6.61235676587701	4.60050298640646
H	-1.15828185569731	-8.73432491369770	5.22222103671575
H	1.14512284713800	-8.43314965468500	5.97867781681580
H	1.28344469325579	-6.80136090555613	5.06854752297528
H	6.66651897682475	-4.13424798233607	1.15175117817965
H	7.33578298164830	-4.53660589425582	-0.45873724542645
H	7.17651593584475	-5.82383462954850	0.78870425286230
H	4.22803062619210	-6.49221267128331	-1.56168700486814
H	5.69213036635690	-7.25322842852683	-0.83707900449844
H	5.85958517576016	-5.98852581930621	-2.10294781389983
H	4.79905227059604	-4.54572315153534	3.55857448103969
H	3.91028212700216	-3.88253236862669	4.97509496281349
H	-1.80876343427644	-5.40457756201049	1.93857160304092
H	-2.36876925438316	-4.55812498712864	3.42606615342730
H	6.61518677299665	-0.08018688529914	0.56642446500223
H	4.82666663834731	-0.11770049685073	0.79116982693605
H	5.76165644574377	-1.59012971400769	1.05092760273838
H	6.94925984259623	-0.82603222502130	-5.45811458134562
H	7.38570967755292	0.57527824040110	-4.43493467384966
H	8.26614513008266	-0.96202402224490	-4.25609208271163
H	-4.45053129665380	-2.20354949337509	-0.68986645191347
H	-3.26815676792438	-3.34592964223584	0.03787114561872
H	-2.87133160623180	-1.62205850388932	-0.05468993686310
H	-4.29767251581711	-1.80681253995956	-5.77047812811099
H	-3.18569849897832	-2.95457299770404	-6.57535665051384
H	-4.59140152598920	-3.55942824562356	-5.65033425975907

IV-SS

104

Coordinates from ORCA-job 4-SS

C	3.86625406613919	-8.22071374597529	-0.15381787928275
C	3.65366168459746	-6.83538751934549	-0.00632803969813
C	3.23159918991559	-6.31100484496257	1.25080595119159
C	3.03917454754145	-7.21426248872475	2.34461624712007
C	3.26460458523940	-8.58460857878771	2.14802510645795
C	3.67956190659384	-9.12157408499157	0.90869880695517
C	3.92781740424285	-5.88472084631826	-1.14144823180746
N	2.77356674605346	-5.04933013188695	-1.60448799489510
C	1.58386591749103	-5.87244774091386	-1.90808323132650
C	0.27297725194647	-5.14803289237524	-1.59817299461305
O	0.24245263910238	-4.66604360534635	-0.23812226419285
Y	2.17210606557434	-3.30890064324893	0.36855278532644
O	4.16226692264869	-2.01096603359943	0.60933690979092

C	4.52001328859745	-1.04561273467423	1.29895706318565
O	5.33849146380625	-0.10850715414155	0.83893383713004
C	5.74047859406803	-0.15843675648069	-0.58325095576400
C	7.03614609267830	0.63218065622465	-0.66743502604668
O	3.00733146979413	-5.01547567360648	1.40427646868400
C	2.60499923067704	-6.65545381900395	3.67323934895781
C	3.92083960417887	-10.60382425992752	0.74634242739253
C	3.25221701110323	-4.25218109580006	-2.77516204518357
C	2.25557898277016	-3.36442420732615	-3.47499286262705
C	1.99095289979461	-3.52207960305030	-4.84963490210664
C	1.12848679177023	-2.65558236060498	-5.54313618901179
C	0.52666986149960	-1.61128375099261	-4.80573016035164
C	0.75200104684171	-1.41612679828154	-3.43423570917489
C	1.63267360451285	-2.30898805335488	-2.74663333586067
O	1.84352193604760	-2.18162093664938	-1.44328226453393
C	0.08206666123594	-0.31562666431026	-2.65797402783485
C	0.85685496189696	-2.81934702718835	-7.02007172009085
C	-0.33792017454775	-5.55443036018011	0.72263882956700
O	0.47547248676750	0.67358447694630	0.59816671885657
C	1.01383779479050	0.36666244252714	1.63713750655483
C	0.27965323348152	-0.28598235453406	2.79732887154197
C	0.77221359494089	-1.73332882269487	3.11919104560065
C	-0.36126100061320	-2.55295819132798	3.75856520176436
O	-1.42064594481775	-2.71263054381445	2.83900133809750
C	-2.53606908368454	-3.38728991851905	3.36462148320046
C	-3.60467121470997	-3.56683344558350	2.32615464120689
C	-3.52479032792460	-3.14118645559003	1.05423096124572
O	1.29828318937590	-2.34812940850619	2.00827491779248
O	2.36486231805930	0.64101234784223	1.74227072165461
C	3.17368697933971	0.42376593654654	2.90171018424333
C	3.97101078528235	1.71549166619804	3.10911952354652
O	4.78034337769282	1.54235759360851	4.25629723360114
C	5.64579099872195	2.63945181127944	4.52857664638180
C	4.91735157662639	3.86939931031907	5.00353181247806
C	5.05364398124577	5.09544812468670	4.47089523313542
C	4.07326655326896	-0.82582532779746	2.72459603010463
C	4.61057924380107	0.38484537761461	-1.44865942944969
H	4.09397455519697	-3.63165363941274	-2.38859368179263
H	3.69715110955351	-4.95078241628572	-3.52660748934208
H	4.72218807343960	-5.16201313943838	-0.84407907161499
H	4.33641696243776	-6.46158269524437	-2.00757655409841
H	1.64751054187188	-6.79072928787610	-1.28851219481576
H	1.56651281444028	-6.20051076697805	-2.97535104647253
H	-0.59104016015007	-5.82720826792798	-1.76575256691677
H	0.14162370546371	-4.25935248826029	-2.24365870958867
H	0.25775282097633	-6.48629277044112	0.83404531394423
H	-1.38197824400110	-5.79827657322454	0.43113482484039
H	-0.35930716613158	-5.00617609598485	1.68238022754153
H	-0.15702035571821	-0.91706492558497	-5.32499844220467

H	2.48492139706996	-4.34524276666061	-5.39512048787917
H	4.19587248957426	-8.60447367237275	-1.13517169793207
H	3.11028151827609	-9.26829895559454	3.00120877922245
H	5.91886408569246	-1.22766271357184	-0.82113029384969
H	4.95855671108284	-0.68369167870400	3.37839903304924
H	3.53338270970086	-1.73830716051057	3.03325314353574
H	2.55139648531103	0.26343725158778	3.80653632110473
H	6.27195386960086	2.88322422847589	3.63503721930630
H	6.32747887391263	2.27437565971353	5.32732266058657
H	4.23850435258941	3.71137217713596	5.86193082863357
H	5.72048496771572	5.27647389237262	3.61031313700936
H	4.51603209768258	5.96690266549326	4.87635965610901
H	-0.77509200070192	-0.32569680194553	2.46777536688742
H	0.32995598429294	0.35259659937128	3.70654217682884
H	1.54215416496962	-1.66193473023415	3.93758686508715
H	-2.96145837979596	-2.83407786168746	4.24486567467233
H	-2.24135248387814	-4.39307846545758	3.76977283152257
H	-4.50938979023406	-4.08978210481619	2.68544923604950
H	-4.35377585895929	-3.30342261354584	0.34832085879807
H	-2.62948892548764	-2.61391111093985	0.68933377437728
H	3.69413433560050	-0.23131669574649	-1.36049534748366
H	4.92525636520552	0.37324045822940	-2.51158583170554
H	4.36880616949340	1.42992805072612	-1.16922968741702
H	7.80564180784317	0.21552262006219	0.01169660032171
H	6.86996263224182	1.69588876953069	-0.40197343769615
H	7.42983125737111	0.59386450003569	-1.70214278036483
H	-0.71682045051076	-2.04276595066962	4.69074518737565
H	0.05259789005555	-3.54813509396850	4.05860884238817
H	4.58885418680362	1.92524664431918	2.20384331651904
H	3.25181801694253	2.55954561906196	3.22746226038246
H	-0.49879900253192	0.35389328785030	-3.32211542883369
H	-0.60616413597569	-0.72322328237269	-1.88679286071751
H	0.81174956591671	0.29046726887992	-2.08362693180518
H	1.35290137393438	-3.72240485721306	-7.42814866957554
H	-0.22982588767977	-2.90969471467246	-7.23294304930423
H	1.22165756686852	-1.94793299597442	-7.60597597351595
H	2.49080778387095	-7.45255567466994	4.43364613526138
H	3.33527580171683	-5.90931141659061	4.05264299481113
H	1.64038867014346	-6.10954700078209	3.58834778567359
H	4.17434509514906	-10.86273943717490	-0.30082213422417
H	4.75751763345083	-10.95828417447882	1.38661646008053
H	3.02920660284077	-11.20191155920842	1.03196726831694

IV-SR

104

Coordinates from ORCA-job 4-SR

C	-1.42890000611835	-2.99487677747233	-4.69454656284642
C	-0.78216635476643	-3.12082550096135	-3.44899912526854

C	-1.51514929507237	-2.92027350913294	-2.24177201872380
C	-2.91081296589245	-2.60855293408649	-2.32911615905418
C	-3.50932451521149	-2.49702071932684	-3.59246873860226
C	-2.79501405627145	-2.68197690829176	-4.79764151812080
C	0.66569275034214	-3.52615906674718	-3.36870049550721
N	1.57250577396810	-2.59880972836829	-2.61627933202980
Y	0.96219394431236	-2.84637506415433	-0.01699091703567
O	2.38842338871247	-4.88756652414423	0.13499400139927
C	3.01459075181493	-5.32771059369932	1.10498988147987
O	4.29020489454132	-5.72170272963419	1.01926104991377
C	4.99922671563184	-5.56410965123598	-0.26096628007299
C	4.77821675552651	-6.81531853157923	-1.10205323448525
O	-0.92340801246570	-3.02661733581563	-1.06637604878163
C	-3.69307901064615	-2.43480572894124	-1.05461048895535
C	-3.48342588279876	-2.55496694450815	-6.13613439048065
C	2.96556738148878	-3.09670403291475	-2.81035928623508
C	4.09754208508198	-2.28420883665291	-2.22774599254815
C	5.19875328532592	-1.93417675501654	-3.03481714012587
C	6.32071770888732	-1.25978402959842	-2.52265502061951
C	6.30515339448045	-0.93124929899188	-1.14822932616990
C	5.23062456284657	-1.24728962584281	-0.30450885866200
C	4.09417558983868	-1.94085859572704	-0.83987965244760
O	3.06701404637672	-2.22816444862449	-0.06843918434984
C	5.21634019981013	-0.87243104114892	1.15327808324035
C	7.49084229041763	-0.88176777305400	-3.40003145860570
C	1.39563931340977	-1.19042369316218	-3.03805081872119
C	1.55343425955642	-0.19197736013598	-1.88970577489096
O	0.68283165646502	-0.50396108291342	-0.78493538049544
C	-0.58990066434354	0.14116394703276	-0.81675105500962
O	0.91582091193322	-1.59373737856694	2.16002543938457
C	1.09717406887068	-2.56133427915464	2.91191551381240
C	-0.03955032203729	-3.17761038577723	3.68373534825915
C	-0.87092983886537	-3.83562638142456	2.51913236504588
C	-1.65196546518748	-5.06162049653718	3.00037572863552
O	-0.78635059022847	-5.98477243566319	3.64141549630802
C	-1.39948022695078	-7.22134348190344	3.91416685428851
C	-0.51521879020111	-8.12902981189343	4.71605660710729
C	0.68877086356089	-7.81431440030085	5.22078343722638
O	0.00657884404198	-4.14028399894056	1.49112508549797
O	2.34625583777096	-3.07095991459768	2.94203501076874
C	2.71306978036709	-4.35700467832033	3.48974804967412
C	4.17718863881409	-4.20907871992675	3.90794001570310
O	4.53912289019930	-5.40115883933767	4.57363268366871
C	5.92972151400029	-5.50932189358484	4.85746318842981
C	6.40199630760213	-4.53821250557299	5.90752017925221
C	7.43572904738524	-3.69254681490965	5.75962520554549
C	2.44849640798989	-5.50946643580903	2.49769832012719
C	6.45476357365501	-5.29871859496840	0.08955420891842
H	2.97535609600997	-4.12401114767827	-2.37967001088250

H	3.15232372067786	-3.21897739855223	-3.90643401201379
H	0.75821702556757	-4.51730230717220	-2.86561669881617
H	1.05877439640538	-3.66589846775238	-4.40574107346928
H	0.37471736076729	-1.09630144259518	-3.46124024352249
H	2.11054830841037	-0.91385443024868	-3.84907031290299
H	1.33290731734453	0.83569327040541	-2.25374862419962
H	2.58076005658866	-0.19811836525653	-1.48406429369989
H	-1.19036891906902	-0.16368466409728	-1.70105033243301
H	-0.45767728322832	1.24545431586744	-0.81333744345762
H	-1.12950773407749	-0.15657857595344	0.10134320745778
H	7.16910487110513	-0.39536308680081	-0.71705297003057
H	5.17734148686772	-2.20676958499594	-4.10481239666375
H	-0.84066490280265	-3.15342479604715	-5.61536373388715
H	-4.58632260624544	-2.25858514153864	-3.64161605261532
H	4.56403483222699	-4.67877327306016	-0.76568581712190
H	2.91518220878347	-6.40499385157963	2.95297416619302
H	1.35460367379155	-5.64519589684942	2.39515821787347
H	2.12024745318750	-4.56811089991774	4.40466841693457
H	6.53388040912241	-5.39415108360464	3.92386462999739
H	6.06581233878401	-6.55151413145921	5.21946040809632
H	5.83619132901556	-4.55937542958453	6.85736025640332
H	8.01071980131469	-3.64876944509805	4.81862721622074
H	7.75537810581868	-3.01961613818974	6.57075338614079
H	-0.59474642738898	-2.37655353778069	4.21137459118052
H	0.28147160531084	-3.94425522098697	4.41162514733094
H	-1.65533146713062	-3.09327352917498	2.20421107397382
H	-1.69442622210445	-7.73645787323692	2.96205942057708
H	-2.36224704745518	-7.07246881251808	4.47342381900250
H	-0.93889032536874	-9.13499720825356	4.88824682088320
H	1.27047196221607	-8.54353580624199	5.80487298431179
H	1.12868412087737	-6.81791455993641	5.06520957226563
H	6.55364416295835	-4.37354644708918	0.69033582352993
H	7.04062602768344	-5.15755378874898	-0.84000704212947
H	6.89263038332757	-6.14625450203463	0.65565969488072
H	3.70270955636162	-6.96292367470444	-1.32154006174730
H	5.16251191439080	-7.71591234977727	-0.58109691279483
H	5.31348076579362	-6.71879348224347	-2.06784731317701
H	4.81687202680437	-4.03324834495504	3.00992682909750
H	4.27451418905314	-3.31227703553160	4.56440680691048
H	-2.12637224988720	-5.52441984521459	2.10232496865859
H	-2.47154952711279	-4.75223434273263	3.69876836753191
H	-2.77481874956125	-2.70808806123267	-6.97421209851220
H	-4.30046463812489	-3.29939621766789	-6.25267415359013
H	-3.94679657320579	-1.55388009277554	-6.27045958696629
H	-4.76528030392746	-2.24512432152892	-1.25725271711677
H	-3.60776341017706	-3.33513622487816	-0.40972768136229
H	-3.30201103414745	-1.59299691649321	-0.44324222198452
H	8.45269871849148	-1.26207443481657	-2.99430008372926
H	7.37857443729562	-1.28716429351634	-4.42531854509827

H	7.60148719646742	0.22081564056927	-3.49129654766274
H	6.12588164429423	-0.30859679432198	1.43917212169671
H	4.32292196773039	-0.26105030821169	1.40084992370640
H	5.13926051220044	-1.77003432016639	1.80399661589066

IV-SS-TS

104

Coordinates from ORCA-job 4-SS-ts

C	3.81104736755174	-8.22121236040568	-0.07056379822347
C	3.89316671074754	-6.86550766239399	-0.44335536194822
C	4.17426470244285	-5.86702901286492	0.53559378821109
C	4.39088795633274	-6.27172892772252	1.89031456172015
C	4.29847250069471	-7.63349381455756	2.21368328576654
C	4.00383035195481	-8.63347225708646	1.25899577013829
C	3.80497719152587	-6.41479757401502	-1.87488302216291
N	2.62337497675751	-5.55454688452592	-2.20704200363456
Y	2.36061894329873	-3.64728212410375	-0.31529499307856
O	4.23843676909920	-4.58229115171687	0.17810327037949
C	4.71252717794414	-5.22020451490965	2.91621572862942
C	3.91038247164573	-10.08604342793175	1.66261944018847
C	2.89524547406593	-4.92712529429488	-3.53931359987582
C	1.91332171037648	-3.90298630784752	-4.04199260504733
C	1.19791815820823	-4.08800143919988	-5.24055763192600
C	0.34055203612563	-3.09758135099755	-5.75177346359270
C	0.23131652846986	-1.89393805627337	-5.01894760815795
C	0.93222578293096	-1.66011536737211	-3.82579860875523
C	1.78884548851850	-2.68457516881571	-3.31064154341793
O	2.45083618430658	-2.51762949549117	-2.17254295494969
C	0.82171011972975	-0.36248443606463	-3.07122854636432
C	-0.41387132373279	-3.29033769456505	-7.04633440361042
C	1.40069105986598	-6.37716608664111	-2.20669025507920
C	0.12077736873739	-5.57337843750884	-2.04022618679054
O	0.25662301542380	-4.76291013513113	-0.86176307395652
C	-0.98629731523617	-4.28869671337427	-0.33091970292164
O	1.62740076855723	-1.32461461966534	0.31055376447616
C	1.56926187730455	-0.88096575554048	1.45696873448003
C	0.78076604428725	-1.55226355023603	2.53894546160791
C	1.24016768769354	-3.04407952833128	2.79234004371488
C	0.18652086424138	-3.72446165434544	3.68514542001910
O	-1.09436701482114	-3.63090585746865	3.08617043513533
C	-2.08455253670891	-4.37591365254522	3.75118535109103
C	-3.44160235284509	-4.17066764751670	3.14594243020152
C	-3.73511235969970	-3.32325231599411	2.14581466116140
O	1.46266230566574	-3.72896901302829	1.63678928828325
O	2.21872875337997	0.28916504906736	1.67701749089647
C	2.67242830825684	0.71838616921811	2.97607037527085
C	3.11953626871378	2.16693259465245	2.77571848569964
O	3.46765220947150	2.67348370487498	4.04755758831464

C	3.99097433065836	3.99805167302347	4.02091339829637
C	2.95894547082884	5.03915158986386	3.67499173879399
C	3.09220067560484	5.95665413681503	2.70232181656195
C	3.80570972863710	-0.20104147150697	3.48596571824405
C	4.61968844053406	-0.75073330939646	2.32455194776098
O	5.64645550767373	0.05434643016872	1.99213962215761
C	6.44553656893206	-0.33088515484769	0.81932352459551
C	7.84130064489601	0.22287348291554	1.06103851565231
O	4.33125107188772	-1.78248078511875	1.73827241104722
C	5.77418186693700	0.19694054212950	-0.44342691672660
H	3.88713159732441	-4.43731722881089	-3.43080108616533
H	3.00870739836895	-5.73981319358487	-4.29822388271891
H	4.69744452528678	-5.79579202285440	-2.10308120501113
H	3.82615446411043	-7.29487840314845	-2.56246553979095
H	1.48149062814158	-7.08000558727434	-1.35099418670849
H	1.32239386561218	-6.99355879741398	-3.13728335412302
H	-0.73047525621836	-6.27659810212461	-1.89499820063794
H	-0.09875694537199	-4.93027242262699	-2.91862029645334
H	-1.69970677260574	-5.13477443336644	-0.22613880151488
H	-1.43264523652618	-3.51645775518247	-0.99581269723372
H	-0.76672023768813	-3.88041729248316	0.67261533822435
H	-0.43049354500357	-1.09648850263271	-5.40050888077477
H	1.32065647747248	-5.03624267165110	-5.79319206230244
H	3.60725276345183	-8.97719028419471	-0.84922946802991
H	4.46513120688944	-7.93272811789829	3.26347652478078
H	6.46007261063871	-1.44035712454630	0.79288925536116
H	4.42860474092865	0.38714374616775	4.18695868313486
H	3.38126885192776	-1.07248338436186	4.02043504983531
H	1.83632706401190	0.71867303624108	3.70894858976410
H	4.85983056138833	4.06806535442678	3.32118845211622
H	4.37312346503945	4.17328402456456	5.04989148144368
H	2.04441353761605	5.02029255758417	4.29621832835785
H	3.99328910093234	5.99157639692222	2.06606141903768
H	2.31634615790649	6.71408653185418	2.50940471429021
H	-0.26325019896009	-1.61067501676799	2.16693723769053
H	0.76607634223039	-0.98327972414471	3.48840230729434
H	2.16860820352587	-2.98773107595491	3.42797328242855
H	-2.12801293210939	-4.09853270950946	4.83888761980413
H	-1.83402127981239	-5.46964912886390	3.74087092241307
H	-4.23893239524383	-4.78544054646992	3.60128786258825
H	-4.76267446006143	-3.22812999496843	1.76307254195722
H	-2.95554363514675	-2.69821006293948	1.68409017272715
H	4.75466314263377	-0.21932116094113	-0.56139717808360
H	6.36371666655355	-0.09933978305942	-1.33415175695942
H	5.71055411851734	1.30443640513970	-0.42456358707395
H	8.27117706152040	-0.17666013626067	2.00044940219739
H	7.82397343118448	1.32997326047875	1.12721496822881
H	8.51066242500169	-0.06258922575832	0.22552568996089
H	0.17267759187399	-3.25645858860994	4.70339294256980

H	0.49041059322181	-4.79149423391746	3.80385662478875
H	3.98716970174733	2.19926137437049	2.07316507184784
H	2.28422583733114	2.73775206722172	2.30664805550271
H	0.10004587634935	0.32779321759527	-3.55062370706058
H	0.51695138816424	-0.52897239461075	-2.01711754662593
H	1.80716830822806	0.14727872095236	-3.01051922775046
H	-0.34392700078688	-4.33589613533302	-7.40736027008657
H	-1.49144971539020	-3.04397929885565	-6.93820162819708
H	-0.02015262853009	-2.63679138764632	-7.85546407660366
H	3.71150988716662	-10.73928576458680	0.78983101435932
H	4.84849968691828	-10.44311682886105	2.13912330974638
H	3.09620159003298	-10.25893580581475	2.39940235404500
H	4.87999627144880	-5.66483867330747	3.91686884254522
H	5.61443401759966	-4.64105013804818	2.62659238240794
H	3.89232254328516	-4.47548091551002	2.98413441018063

“IV-SR-TS” (see above)

104

Coordinates from ORCA-job 4-SR-ts

C	3.85882647082818	-2.42442425836365	-1.50916346832264
C	3.49855341482741	-2.95530327905076	-2.78265435824274
C	4.43915720537074	-2.96256821398068	-3.82931829057448
C	5.74404973716818	-2.46353729060840	-3.66185961206098
C	6.07808845772406	-1.92918097280684	-2.39785254287897
C	5.17136225327782	-1.88893808474870	-1.32658810776349
C	2.12767124683881	-3.55656460159294	-2.96336446896486
N	0.95187169574642	-2.66364266204855	-2.69194694638908
C	1.02821814998881	-1.36048387835666	-3.39487474784137
C	1.65200208811542	-0.24985478838242	-2.54380216880233
O	0.97914337036871	-0.09341912281524	-1.27765563365067
C	-0.11060102012564	0.83011704193506	-1.29621890187544
C	6.75870469673216	-2.50999474340886	-4.77998769403739
C	5.51397533296647	-1.26648807945739	0.00081167043120
O	2.97123652887180	-2.38430141425718	-0.52969499805783
Y	0.85548954289965	-2.37409692535144	-0.15884489694650
O	0.39473350313310	-4.22347838895547	0.83278751147330
C	-0.61941403043676	-4.25734410971893	1.78722155617524
C	-1.24296576687963	-5.64958337517511	1.93674820586866
O	-0.36585220508527	-6.53561627979578	2.61217155897500
C	-0.75658279839490	-7.88548185809695	2.51757967528706
C	0.01664472755710	-8.76666577463943	3.45313057017689
C	0.87107596624398	-8.35136497912368	4.40228963814725
C	-0.29276525649373	-3.42884910121259	-3.04558898725761
C	-1.59260012081268	-2.66471485332161	-2.98478128666935
C	-2.42977684797009	-2.59807074135122	-4.11702773652156
C	-3.68422202674078	-1.96571906905083	-4.08500413036698
C	-4.08707667175993	-1.39011131366118	-2.85953267971199
C	-3.28981257127621	-1.42417421112568	-1.70608937678594

C	-2.01037217092928	-2.06492109860170	-1.75750394475634
O	-1.23053783229731	-2.09381618462108	-0.68833949694599
C	-3.74350845270775	-0.82263272536936	-0.40278009424289
C	-4.57754569862520	-1.90894966941070	-5.30164463972298
O	0.92525650725889	-1.79072607797723	2.16340345692663
C	1.10691425547978	-2.84274704202734	2.80657020161786
O	2.36826310897798	-3.14382970807460	3.11348435059682
C	2.79154266934512	-4.39218461141732	3.73138748994106
C	2.93962669382959	-5.51680153619934	2.69968010099906
C	3.90161258308040	-5.34314110355910	1.53161928068770
O	5.17567757132022	-5.10877512615293	1.95182781695151
C	6.21257600963968	-5.03163876231955	0.92212814034349
C	7.37208232320012	-4.26455561358142	1.54153547542076
O	3.59172378137746	-5.47438613615977	0.36361758243404
C	6.59263352124600	-6.43796606850358	0.46762658105017
C	-0.05259374560685	-3.73852824617899	3.16439333086680
C	4.04627224157375	-4.03144107778040	4.52963581776124
O	4.42218292705732	-5.19598079691318	5.24129666673961
C	5.72035881825915	-5.15343044965765	5.80000214563100
C	5.82210590287170	-4.43165197280126	7.12112954867322
C	4.77735295076125	-4.04684751938832	7.87223669984769
H	2.01389829901399	-4.43274450020553	-2.28299212951661
H	2.04062189644785	-3.95010067571649	-4.00492244994863
H	-0.32304590146207	-4.29588889945317	-2.34563052952386
H	-0.17675274691251	-3.85821418628762	-4.06980822135191
H	-0.00715557974700	-1.07159909033125	-3.66844782066331
H	1.60612218867263	-1.44531519310450	-4.34469659418417
H	1.61923501847414	0.71172225261860	-3.10252377356299
H	2.70895564999175	-0.46935045315445	-2.30703473863726
H	-0.91111048749627	0.51811315365801	-2.00136370289982
H	0.25362410790249	1.84544121437046	-1.56802546360636
H	-0.53401077549133	0.86044796778854	-0.27525452841159
H	7.08951555526286	-1.51371420662200	-2.24404779124053
H	4.14294587618491	-3.38071220684258	-4.80716656062804
H	-2.08747034846975	-3.06743288957782	-5.05582254216487
H	-5.07093885998788	-0.89255065860235	-2.80081737778823
H	5.78441598099311	-4.47007603858737	0.06512765773444
H	3.28409447203864	-6.39914430494678	3.27996871685177
H	1.94902300691325	-5.75383691267082	2.26702178874192
H	2.02087634619307	-4.71585949577612	4.46208125378228
H	6.44575105508193	-4.71373528224488	5.07102415107530
H	6.03497853750470	-6.21329709611621	5.94019068894430
H	6.85358971536335	-4.24540841146961	7.47343535675802
H	3.74394735420464	-4.23988872352690	7.54216488667240
H	4.91922815381190	-3.53657095392699	8.83692533956610
H	-0.80290973197850	-3.12585922625220	3.70445559789009
H	0.23737212075293	-4.59129960127405	3.80182158521024
H	-1.47105067089418	-3.58581905460120	1.49665654292154
H	-0.63785317379673	-8.25851172390493	1.46690252308385

H	-1.85011405806621	-7.99781863452591	2.74672690047748
H	-0.17708934094837	-9.84647504902540	3.32076394946890
H	1.39190195331410	-9.06836123553128	5.05488410325901
H	1.07435380932204	-7.28073618108579	4.55437602506409
H	7.05510654755317	-3.25554767003969	1.86968249244147
H	8.18404331295117	-4.14154291405750	0.79748421066045
H	7.78597812927707	-4.80759266989640	2.41649405671648
H	5.72292266297600	-6.94986831178736	0.01416746985537
H	6.96507241799664	-7.04066600624757	1.32155679157833
H	7.39429846467773	-6.38575622268983	-0.29637582209116
H	4.85467749274674	-3.70399369082205	3.83946014370053
H	3.80441196012978	-3.18242133013008	5.21124302917498
H	-1.46279144587541	-6.01606627966180	0.90636661119848
H	-2.21586329592444	-5.58021510401711	2.48765662672180
H	6.59243280345282	-1.02447530398880	0.07476936971438
H	4.93949237032425	-0.32864020131262	0.16572442379398
H	5.23220580888739	-1.93375691641936	0.84131080929731
H	6.28034890583551	-2.72485104847059	-5.75635605016015
H	7.30883432851531	-1.55079692100754	-4.87841865261879
H	7.52403675664407	-3.29923729232054	-4.61080183999982
H	-4.09205675829557	-2.36957849567077	-6.18476433043420
H	-5.53709318338862	-2.44424887114505	-5.13424380249803
H	-4.84154684379302	-0.86432430562364	-5.57281726107700
H	-4.75697160453842	-0.38425693367188	-0.48717178807576
H	-3.75602961045982	-1.58343326910365	0.40669674247898
H	-3.04915667968106	-0.02855708976963	-0.05335893738408

V-SS

104

Coordinates from ORCA-job 5-SS

C	2.10039948744445	-3.69369442446803	-2.28467592676650
C	2.70375056546799	-4.89641592638464	-2.75444407637521
C	2.51414045616411	-5.30731411750522	-4.08829969965095
C	1.72858758916100	-4.56523498365605	-4.98773721721351
C	1.13112545303090	-3.37979957683239	-4.50242749308042
C	1.29568975194461	-2.92589432663665	-3.18439240868587
C	3.59857403278740	-5.66330794363115	-1.81631575437667
N	2.97548632223132	-6.24626824311476	-0.58789735517594
C	1.97218328924167	-7.28415339736061	-0.88326974488308
C	0.60164185092211	-6.73851211206608	-1.26147361309152
O	0.17254527330301	-5.78998867367448	-0.26651186281155
C	-1.19747064407476	-5.39900741575853	-0.41485683418529
C	1.54176830645428	-4.99719531678041	-6.42313099209249
C	0.64158943195680	-1.66667190253180	-2.68180832278914
O	2.26323310251280	-3.30893399139150	-1.02241458576459
Y	1.77544453464934	-4.31490108121562	0.83583730639237
O	0.04579262143322	-3.36748524731966	1.65607912168582
C	-0.09649033731430	-2.47410639367065	2.71139828042358

C	-1.57288774357354	-2.09311000046266	2.96310971447431
O	-2.12304250724903	-1.18744207760738	2.02484399429294
C	-2.50954403040239	-1.74103908557127	0.78350128717906
C	-3.29945545643164	-0.75057553444123	-0.01978540712172
C	-3.63165082571707	0.48558292971845	0.38660740785897
C	4.09584554835984	-6.80181913408433	0.24307542786227
C	3.71641078679911	-7.53837693536658	1.50100475381299
C	4.11859947358862	-8.87410517613232	1.70337652243509
C	3.85281620949625	-9.55844398676213	2.90121190971974
C	3.15895199165604	-8.85397297198890	3.91054171287371
C	2.73524401492482	-7.52609516832774	3.75615180825005
C	3.01167758086628	-6.84773565136064	2.52865946155570
O	2.60491722487441	-5.59722532124645	2.34532088149631
C	1.99428542824633	-6.78810984456474	4.83834415187262
C	4.29299921943133	-10.98740278654421	3.11502110503168
O	2.73174924690593	-2.40564077631688	1.84501281455770
C	2.18185708495630	-1.36402804422824	2.23088050159715
O	2.89010876527095	-0.24879675092096	2.43667364885274
C	4.27689302914125	-0.22909848461030	1.99572203051269
C	4.35740362749726	-0.09668321631561	0.46350916963926
C	3.43193502829948	0.97737513233885	-0.07834091677503
O	4.05674446717057	2.17731276680821	-0.17524312969244
C	3.26055756276962	3.30431733426635	-0.65940573792990
C	2.51859218473644	3.94008107588325	0.51190621966040
O	2.26151098004544	0.79237524843519	-0.36635174102439
C	4.22995320962901	4.24295886323377	-1.36216843736831
C	0.71584547749130	-1.17556949288656	2.48155464906642
C	4.92274680553902	0.92358858873130	2.76232721909006
O	6.29845479842678	0.90920198128874	2.44619406036651
C	7.02543007609561	2.01736077782703	2.96420924717192
C	7.16105775338308	1.99440208838168	4.46417640060279
C	6.84066514942663	3.01409900215545	5.27858076241767
H	4.39561326670499	-4.98119668387434	-1.44491995179369
H	4.11092457045828	-6.48199977793115	-2.37966027498248
H	4.73760798442537	-5.92778056747016	0.49872891902703
H	4.72012140898128	-7.47520994491744	-0.39369155332851
H	1.87025056820395	-7.90496792643529	0.03098283997798
H	2.31184257850417	-7.96706635926118	-1.70203594027897
H	-0.12414078868042	-7.58339021338678	-1.28760557902560
H	0.60165191934884	-6.24474973449125	-2.25656302861707
H	0.50673891149225	-2.77910447915943	-5.18687099298682
H	3.00159695604683	-6.23598896907914	-4.43353324038472
H	4.66617834763132	-9.39106679776706	0.89607089599821
H	2.93643843098887	-9.36663679619152	4.86267337699303
H	2.52029182967049	2.89119604225804	-1.37622376597724
H	5.41215935199653	0.13213860307410	0.21797554049943
H	4.06049428831839	-1.05410371660107	-0.00715946217230
H	4.76139799459908	-1.18161486004139	2.29253791288407
H	6.56817738525589	2.98189737752876	2.63137282761962

H	8.03004482717693	1.94270433408118	2.49434408830584
H	7.56785870620092	1.05653538559170	4.88555970147162
H	6.42861578175633	3.95781031560352	4.88131299572402
H	6.98715893376247	2.95404671884290	6.36847044659198
H	0.31415010314701	-0.66196539733223	1.57802815967357
H	0.59584272481964	-0.44777916119444	3.31022592849157
H	0.25873896896653	-2.92756443103259	3.67949902435318
H	-3.12747116586809	-2.66435483566473	0.94574710935888
H	-1.62191595913363	-2.08209964205941	0.19652231814787
H	-3.60061862644883	-1.10877314191264	-1.02094359672835
H	-4.20803499806128	1.16496109884091	-0.25973171972201
H	-3.32860170358932	0.84584770884712	1.38142686827567
H	1.83986549636982	3.20642908188222	0.98830188483192
H	1.90400755767973	4.79250223017751	0.15867193015426
H	3.23122515883075	4.32065679678743	1.27254856354424
H	4.75134645982571	3.72588092063065	-2.19129204997059
H	4.99456427374687	4.62576039150788	-0.65559094159132
H	3.68339967514147	5.11006854860044	-1.78336431843548
H	-1.65995284342105	-1.59234038683038	3.95197233660029
H	-2.16473177664370	-3.03963153881940	3.00122656895629
H	4.45088466208715	1.89349067271496	2.47093644239204
H	4.73915133115661	0.77917623435154	3.85348414871301
H	-1.39050933420036	-4.64228952683584	0.36895791788427
H	-1.86295435869230	-6.27949451211268	-0.27865237566910
H	-1.37025536914027	-4.95983169720647	-1.42209317871150
H	1.85111993567055	-7.41897912908081	5.73715789477518
H	2.53549534691470	-5.86574647379952	5.13854232414650
H	0.99672240380224	-6.44953903962788	4.48476277589125
H	4.79232259293238	-11.39870500375348	2.21537963848196
H	5.00806353897652	-11.07635779096739	3.96114671837370
H	3.43573149159099	-11.65247656416757	3.35451151694881
H	0.12011680946258	-1.12691560832865	-3.49633541029467
H	-0.10378542147415	-1.88684167366835	-1.88555912555878
H	1.37301086650617	-0.97987185356999	-2.20794180300323
H	1.97324287778721	-6.00135990648549	-6.60644262571571
H	0.46872284472007	-5.03614580110454	-6.70733097915461
H	2.03080493472554	-4.29405879449006	-7.13202001488258

V-SR

104

Coordinates from ORCA-job 5-SR

C	-3.07676164519261	-3.60186794801650	-4.18893399814832
C	-2.01971990415769	-3.14339901048795	-3.37715843641215
C	-2.20129164310712	-1.99012842460295	-2.56061294649848
C	-3.46642243730447	-1.32436563312269	-2.57488823602842
C	-4.48904999992617	-1.82268163079032	-3.39485886126880
C	-4.32607735461729	-2.96017564471507	-4.21697747349354
C	-0.72393662365281	-3.90699943919554	-3.30183632339869

N	0.53404953893296	-3.15740010517662	-3.63318887849562
Y	0.93057450493220	-1.33520187119048	-1.71842495999855
O	0.92537960538189	-1.59638184962073	0.63520121965318
C	1.12956850783908	-0.71661575601934	1.48728271121355
C	0.81885924357428	0.72990492491727	1.29299510497760
C	1.66152366185260	1.32092614272784	0.10033707949533
C	1.32203503083346	2.81205262862162	-0.04488036409522
O	-0.06768160708930	2.99386168668865	-0.20968877578028
C	-0.43947635187348	4.33768786010928	-0.38099202027019
C	-1.92784668954960	4.49576993497417	-0.48225554771963
C	-2.82145675602854	3.49733281016722	-0.39567956970346
O	-1.20719129921390	-1.53127459421039	-1.81108008928129
C	-3.65081530300523	-0.10511713462405	-1.71306300311009
C	-5.45726623267666	-3.45929931968685	-5.08463999437198
C	1.64141888703441	-4.15979849627691	-3.64357546119321
C	3.05165918402213	-3.63671712107029	-3.72762509011464
C	3.89106128963255	-3.97013554910307	-4.80845140230448
C	5.22754056218386	-3.53946996946230	-4.87196669518785
C	5.70714393889923	-2.76161391921105	-3.79429264814592
C	4.91446354223075	-2.41732599646952	-2.68824489081215
C	3.55173233857656	-2.85503447180697	-2.64490348768319
O	2.76014282736165	-2.53048263353066	-1.62516729568364
C	5.46150312106541	-1.61605265921649	-1.53758465850201
C	6.12699565711959	-3.90115798822739	-6.03036655011678
C	0.39697733371751	-2.42470994529130	-4.90373715671822
C	1.42911157003480	-1.32248365926885	-5.10302983994590
O	1.46911472483491	-0.48122412737581	-3.93742315800221
C	2.34357979354533	0.64469869346779	-4.08951756803069
O	1.46054382224909	0.61565972155407	-1.06573811574977
O	1.70396004197712	-1.00714935601439	2.65861906177062
C	2.23827504035141	-2.34823207882826	2.83745684926154
C	3.55165603111996	-2.52745670282709	2.05447272795206
C	4.52467539017265	-1.38004951651925	2.26708491897286
O	4.46307567803043	-0.31502950512157	1.67354626070273
C	2.37777856145842	-2.52061742938608	4.34901172990752
O	2.77756591135348	-3.85420693143270	4.58008943710829
C	3.08042012320269	-4.14265388239374	5.93966583147047
C	1.87001616315050	-4.13485571037932	6.83642582998457
C	1.76690884202156	-3.43581924154009	7.97940247247963
O	5.44777507697560	-1.68754516800283	3.20963787161646
C	6.49282594674960	-0.72203483454133	3.56439562408788
C	5.91058823371833	0.52828660314008	4.22037047135044
C	7.42024392836230	-0.43890109889496	2.38461301204077
H	1.53143013014467	-4.72800951348682	-2.69350857606623
H	1.46254087911280	-4.88384455668130	-4.47663626112354
H	-0.57363770280116	-4.29688564289506	-2.26847128858016
H	-0.79786971592896	-4.80186911849757	-3.96675385726103
H	-0.61860435355752	-1.97741293212898	-4.91117998113931
H	0.45103194236059	-3.11124607911348	-5.78639276828688

H	1.13030718653452	-0.70655526312793	-5.98247990886889
H	2.44668095485130	-1.72741612565198	-5.28859234878341
H	1.98370224508111	1.29845160997499	-4.91391961868051
H	3.37775446540055	0.30143750019098	-4.31203828512794
H	2.31810219994652	1.18568651195014	-3.12461237748590
H	6.75386351619605	-2.41054668821887	-3.81491681156592
H	3.48240432368407	-4.58934812668145	-5.62635748115173
H	-2.91562286451963	-4.49764683492096	-4.81385460989647
H	-5.46015274147651	-1.29738804806666	-3.39614975013245
H	7.05881590201168	-1.29298189679544	4.32958984900121
H	3.99554653545333	-3.48250115060018	2.39405760252568
H	3.33199320811693	-2.58632366802638	0.96887064324548
H	1.50021036592880	-3.08136803865927	2.45239428638217
H	3.85640361447664	-3.43935288102723	6.33160445899319
H	3.52848809985778	-5.15979210510739	5.92162033689609
H	1.03129049144932	-4.77207219550864	6.50003894911042
H	2.58885684020440	-2.78923389681546	8.33231749430052
H	0.86758881178126	-3.48911335167144	8.61291133587646
H	1.01687247090369	1.28485462609851	2.22907742752473
H	-0.24995375673464	0.84067910250716	1.01764767037931
H	2.73481298757231	1.28212685150558	0.42140631379978
H	0.04238721956858	4.77196603758430	-1.29798149591127
H	-0.06160924996300	4.96832162776302	0.46953622931066
H	-2.26686403602649	5.53616685616937	-0.63651141426778
H	-3.90191178738596	3.69029809099051	-0.47900952606975
H	-2.49411251510851	2.45722068658072	-0.24761551570717
H	7.77894984811529	-1.38580724337307	1.93445268346083
H	8.30577088553047	0.12672720347242	2.73863554120366
H	6.90916380632988	0.15481208612182	1.60389957933152
H	5.24127307653695	0.25617226834709	5.06113379138744
H	5.34023951691657	1.13365323064800	3.49154143477315
H	6.73360238692295	1.14801681090413	4.63027616668202
H	3.12866448066163	-1.79768873022761	4.75347436924679
H	1.39978201780287	-2.28414636105586	4.83158495095907
H	1.68794754086858	3.37302525907572	0.85430549746488
H	1.88236112247262	3.20316685267371	-0.93005729706948
H	-4.68559389923412	0.28477057373167	-1.77518551627663
H	-3.41961577099048	-0.32627511235417	-0.64946465378258
H	-2.95370686638101	0.70764594459541	-2.00948665429506
H	-5.15826105545244	-4.35161431586045	-5.66968217582076
H	-6.34688664316141	-3.74041998979587	-4.48091533541195
H	-5.79672093880778	-2.68560397210999	-5.80650398833621
H	5.57753558832431	-4.46064741211060	-6.81331627589091
H	6.56744723517942	-3.00066785081183	-6.50945511974617
H	6.98023933269027	-4.53607833933305	-5.70735842738802
H	6.46939238869672	-1.21604740268510	-1.76422957051344
H	4.79410122910414	-0.77379799912671	-1.26190506179259
H	5.54381224363662	-2.23927854107473	-0.62068437720506

