Brønsted Acid Catalysis – Structural Preferences and Mobility in Imine/Phosphoric Acid Complexes

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Supporting Information

Experimental data

Deuterated solvents were purchased from Deutero or Sigma Aldrich Where dry solvents were essential, CD_2Cl_2 was freshly distilled over CaH_2 and Toluene-d8 was refluxed over Na/Benzophenone under Argon atmosphere. Freon mixtures were prepared from $CDCl_3$ and $SbCl_5/SbF_3$ according to literature procedures and stored in small lecture bottles.[1,2] The catalysts were purchased from Sigma Aldrich or synthesized from the bisphenols according the procedure of Klussmann et al.[3]

High resolution mass spectra were measured by the central analytics division in the Institute of Organic Chemistry. Gas chromatography coupled with a mass selective detector was performed on an Agilent 6890N Network GC-System.

Synthesis of Ketimines

Imines were synthesized by refluxing aniline and the corresponding ketone over activated molecular sieves 4 Å in toluene. The toluene was used either in p.A. quality or was dried by refluxing over sodium.

(*E*)-1-(4-methylphenly)-N-phenylethan1-imine **[2a]**
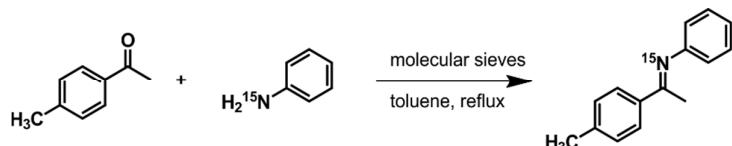
Molecular sieves 4 Å (1.6 g) were weighed in to a 25 ml Schlenk flask equipped with a reflux condenser. The setup dried at 350°C under reduced pressure. 4-Methylacetophenone (0.403 g, 3.00 mmol, 0.40 ml) and Aniline (98% ^{15}N, 0.30 ml, 0.310 g, 3.30 mmol) were dissolved in 5 ml anhydrous Toluene under argon atmosphere. A drying tube filled with $CaCl_2$ was added to the setup and the solution was refluxed for 20 h. After cooling down to r.t., the yellow solution was filtered and the solvent was removed under reduced pressure. The obtained yellow solid was recrystallized in methanol and yielded as a yellow solid (0.123 g, 0.58 mmol, 20 %) predominantly as *E*-Isomer (>99 % via ^{1}H-NMR analysis).

^{1}H-NMR (400.1 MHz, CD_2Cl_2) δ_H = 7.86 (m, 2H), 7.34 (m, 2H), 7.25 (m, 2H), 7.06 (m, 1H), 6.76 (m, 2H), 2.40 (s, 3H) 2.18 ppm (d, $^3J_{HN}$ = 1.76 Hz, 3H)

^{13}C-NMR {^{1}H} (100.6 MHz): δ_C = 165.3 (d, $^1J_{NC}$ = 7.0 Hz), 152.4 (d, $^1J_{NC}$ = 1.6 Hz), 137.3 ($^2J_{NC}$ = 8.3 Hz), 129.34, 129.29 (d, $^3J_{NC}$ = 3.2 Hz), 127.5 (J_{NC} = 3.2), 123.3, 123.9, 119.7 ($^2J_{NC}$ = 2.3 Hz), 21.5, 17.4 ppm (d, $^2J_{NC}$ = 2.8 Hz)

^{15}N-NMR (40.5 MHz): δ_N = 328.9 ppm

HR-MS (ESI, *m/z*): found 211.1248 (M+H)+ (calculated for 211.1248 for $C_{15}H_{16}[^{15}N]O$); Diff(ppm) = -0.37

(E)-1-(4-methoxyphenyl)-N-phenylethan-1-imine (98% 15N) [2b]
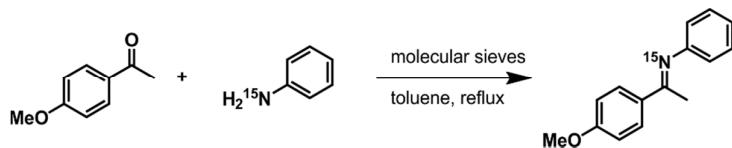
Molecular sieves 4 Å (1.6 g) were weighed in to a 25 ml Schlenk flask equipped with a reflux condenser. The setup dried at 350°C under reduced pressure. 4-Methoxyacetophenone (0.450 g, 3.00 mmol) and Aniline (98% ^{15}N, 0.30 ml, 0.310 g, 3.30 mmol) were dissolved in 5 ml anhydrous Toluene under argon atmosphere. A drying tube filled with $CaCl_2$ was added to the setup and the solution was refluxed for 20 h. After cooling down to r.t., the yellow solution was filtered and the solvent was removed under reduced pressure. The obtained yellow solid was recrystallized in methanol and yielded as a yellow solid (0.223 g, 0.986 mmol, 33 %) predominantly as E-Isomer (>99 % via ^{1}H-NMR analysis).

^{1}H-NMR (400.1 MHz, CD_2Cl_2) δ_H = 7.95 (m, 2H), 7.35 (m, 2H), 7.07 (m, 1H), 6.96 (m, 2H), 6.77 (m, 2H), 2.18 ppm (d, $^3J_{HN}$ = 1.76 Hz)

^{13}C-NMR {^{1}H} (100.6 MHz, CD_2Cl_2): δ_C = 164.5 (d, $^1J_{NC}$ = 7.1 Hz), 161.9, 152.5 (d, $^2J_{NC}$ = 1.7 Hz), 132.5 (d, $^1J_{NC}$ = 8.4 Hz), 129.2, 129.1 (d, $^3J_{NC}$ = 3.3 Hz), 123.2, 119.8 (d, $^2J_{NC}$ = 2.3 Hz), 113.8, 55.7, 17.2 ppm (d, $^2J_{NC}$ = 2.7 Hz)

^{15}N-NMR (40.5 MHz, CD2Cl2): δ_N = 325.5 ppm

HR-MS (ESI, *m/z*): found 227.1198 (M+H)+ (calculated 227.1197 for $C_{15}H_{16}[^{15}N]O$); Diff(ppm) = 0.49

(E)-N-phenyl-1-(4-(trifluoromethyl)phenyl)ethan-1-imine (98% 15N) [2c]
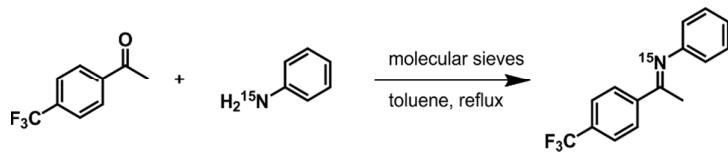
Molecular sieves 4 Å (1.6 g) were weighed in to a 25 ml Schlenk flask equipped with a reflux condenser. The setup dried at 350°C under reduced pressure. 4-Trifluoromethylacetophenone (0.376 g, 2.00 mmol) and Aniline (98% ^{15}N, 0.20 ml, 0.207 g, 2.20 mmol) were dissolved in 5 ml anhydrous Toluene under argon atmosphere. A drying tube filled with CaCl$_2$ was added to the setup and the solution was refluxed for 20 h. After cooling down to r.t., the yellow solution was filtered and the solvent was removed under reduced pressure. The obtained yellow solid was recrystallized in methanol and yielded as a yellow solid (0.340 g, 1.29 mmol, 64 %) predominantly as E-Isomer (>99 % via ^{1}H-NMR analysis).

^{1}H-NMR (400.1 MHz, CD$_2$Cl$_2$): δ_H = 8.11 (m, 2H), 7.73 (m, 2H), 7.38 (m, 2H), 7.12 (m, 1H), 6.80 (m, 2H), 2.25 ppm (d, $^3J_{NH}$ = 1.8 Hz, 3H)

^{13}C-NMR {^{1}H} (100.6 MHz): δ_C = 164.5 (d, $^1J_{NC}$ = 7.1 Hz), 151.7 (d, ^{1}JNC = 1.5 Hz), 143.2 ($^2J_{NC}$ = 7.3 Hz), 132.1 (q, $^2J_{FC}$ = 32.4 Hz) 129.4, 128.0 (d, $^3J_{NC}$ = 3.2 Hz),125.6 (q, $^4J_{FC}$ = 3.8 Hz), 124.6 (q, $^1J_{FC}$ = 272.0 Hz), 123.9, 119.5 ($^2J_{NC}$ = 2.3 Hz), 17.5 ppm (d, $^2J_{NC}$ = 2.8 Hz)

^{19}F-NMR {^{1}H} (376 MHz, CD$_2$Cl$_2$): δ_F = - 63.1 ppm

^{15}N-NMR (60.8 MHz, CD$_2$Cl$_2$, 300 K): δ_N = 338.2 ppm

GC-MS (EI, 70 EV): m/z (RT) = 264.1 [M+] (8.794 min)

HR-MS (ESI, m/z): found 265.097 (M+H)+ (calculated 265.0965 for C$_{15}$H$_{13}$F$_3$[^{15}N]); Diff(ppm) = 1.89

(E)-N-(4-methoxyphenyl)-1-(4-(trifluoromethyl)phenyl)ethan-1-imine [3a]
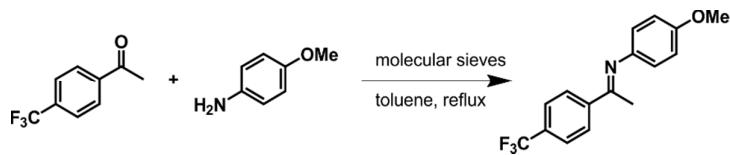
Molecular sieves 4 Å (1.6 g) were weighed in to a 25 ml Schlenk flask equipped with a reflux condenser. The setup dried at 350°C under reduced pressure. 4-Trifluoromethylacetophenone (0.565 g, 3.00 mmol) and Anisidine (0.406 g, 3.30 mmol) were dissolved in 5 ml anhydrous Toluene under argon atmosphere. A drying tube filled with $CaCl_2$ was added to the setup and the solution was refluxed for 20 h. After cooling down to r.t., the yellow solution was filtered and the solvent was removed under reduced pressure. The obtained yellow solid was recrystallized in methanol and yielded as a yellow solid (0.612 g, 2.09 mmol, 70 %) predominantly as E-Isomer (>99 % via ^{1}H-NMR analysis).

^{1}H-NMR (400.1 MHz, $CDCl_3$): δ_H = 8.00 (d, $^3J_{HH}$ = 8.2 Hz, 2H), 7.63 (d, $^3J_{HH}$ = 8.2 Hz, 2H), 6.86 (d, $^3J_{HH}$ = 8.2 Hz, 2H), 6.70 (d, $^3J_{HH}$ = 8.1 Hz, 2H), 3.76 (s, 3H), 2.22 ppm (s, 3H)

^{13}C-NMR {[1]H} (100.6 MHz): δ_C = 127.5, 125.3, 120.8, 114.3, 55.5, 17.4 ppm

Sample preparation

Preparation of binary complexes in CD_2Cl_2

Catalyst **1c** was dried for 30 min at 150°C under reduced pressure. Ketimine and **1c** were directly weighed into a 5 mm NMR tube under an inert argon atmosphere. CD_2Cl_2 (0.6 ml) and 1.0 ml of tetramethylsilane atmosphere were added to the tube. The sample was stored in an -80°C freezer. A 1:1 ratio of catalyst/ketamine was used for all samples. A concentration 50 mmol/L was used for samples **2a/1c** and **2b/1c**. For samples **2c/1c** and **3a/1c** a concentration of 25 mmol/L was used, due to the limited solubility at low temperatures.

Preparation of binary complexes in freonic solvent mixtures

Catalyst **1c** was dried for 30 min at 150°C under reduced pressure. Ketimine and **1c** were directly weighed into a heavy wall NMR tube equipped with a J. Young valve under an inert argon atmosphere. 1.0 ml of tetramethylsilane atmosphere were added and the sample was connected to a vacuum line. The NMR tube was evacuated and cooled down to 77 K. The freonic solvent mixture was condensed through column filled with P_2O_5 and KOH into the NMR-tube.

Solvent screening

Toluene, dichloromethane, and a freonic solvent mixture of CDF_2Cl and $CDFCl_2$ were chosen as solvents, because of their low melting points (toluene: 178 K, CD_2Cl_2: 176.5 K, $CDF_2Cl/CDFCl_2$: <110 K). Vastly superior linewidths and signal dispersion was observed in CD_2Cl_2 and the freonic solvent mixture (see figure 1). The investigated reaction is reported to work in toluene, as well as dichloromethane, with toluene having superior yields.[4,5]
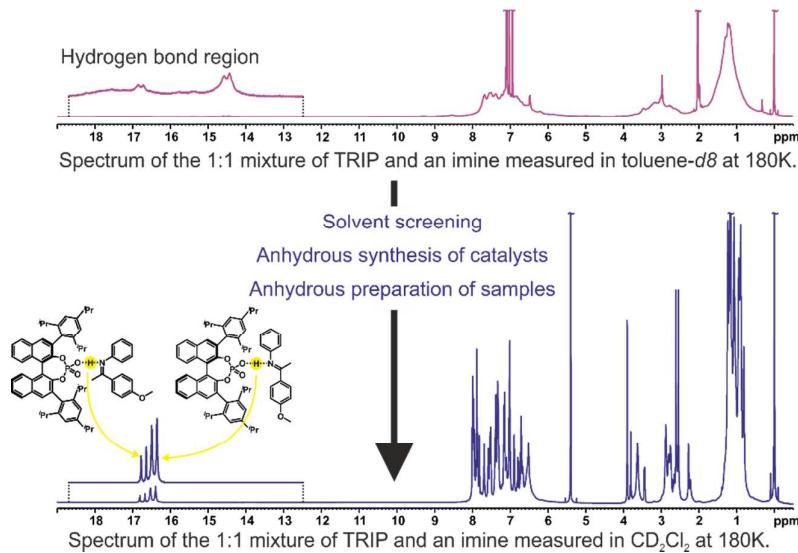
Figure S1: Comparison of ^{1}H spectra of an imine/catalyst complex at 180 K

The observed signal pattern in the freonic solvent mixture is similar to that observed in dichloromethane. Dichloromethane was used as a solvent for most NMR investigations, due to its better solubility.

Identification of the *E*- and *Z*-imines inside the complex

To identify the *E*- and the *Z*-imine inside the complex, standard 2D ^{1}H,^{1}H-NOESY experiments were performed at 180 K.
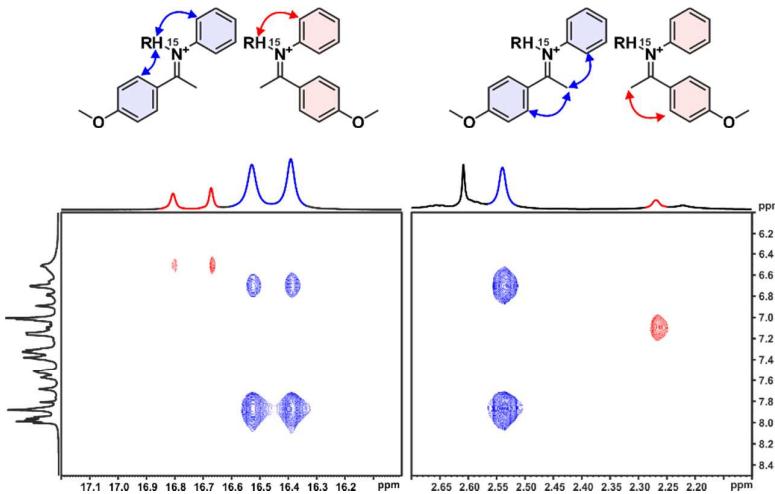
Figure S2: Details of the 2D ^{1}H,^{1}H-NOESY spectrum at 180 K *in dichloromethane*, that was used to identify the E- and the Z-imine inside the imine/catalyst complex. The same pattern was found for every investigated imine.

For the *Z*-imine, the proton inside the hydrogen bond shows only one strong NOE to the aniline part of the imine, whereas for the *E*-imine, an NOE to the aniline part of the imine, as well as an NOE to the acetophenone part of the imine can be found. The methyl group of the *Z*-imine shows only one strong NOE to the acetophenone part of the imine, whereas for the *E*-imine, NOEs to the aniline part and the acetophenone part can be observed (see figure 2). For every investigated imine, the same NOE pattern can be observed.

Assignment of the ^{1}H and ^{13}C chemical shifts

The ^{1}H (black) and ^{13}C (green) chemical shifts of all investigated complexes were assigned with standard 2D NMR experiments (^{1}H,^{1}H COSY, ^{1}H,^{1}H TOCSY, ^{1}H,^{1}H NOESY, ^{1}H,^{13}C HSQC, ^{1}H,^{13}C HMBC) at 180 K. Due to signal overlap, the 2,4,6-triisopropylphenyl groups could not be assigned in most cases. The ^{19}F (orange) and ^{15}N (blue) chemical shifts were assigned with ^{1}H,^{19}F HMBC and ^{1}H,^{15}N HMBC spectra respectively.

Complex 2a/1c

E-2a/1c
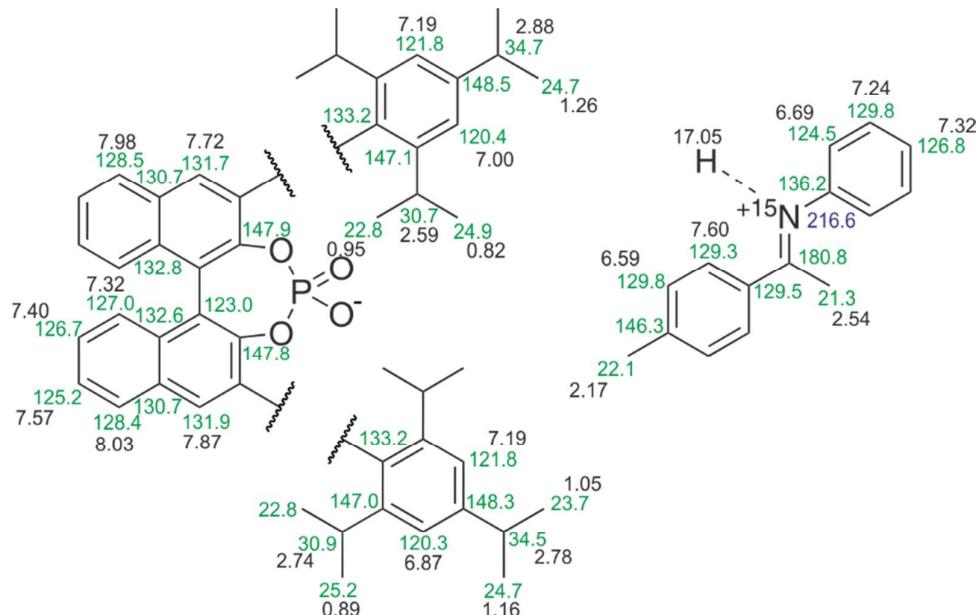
Z-2a/1c
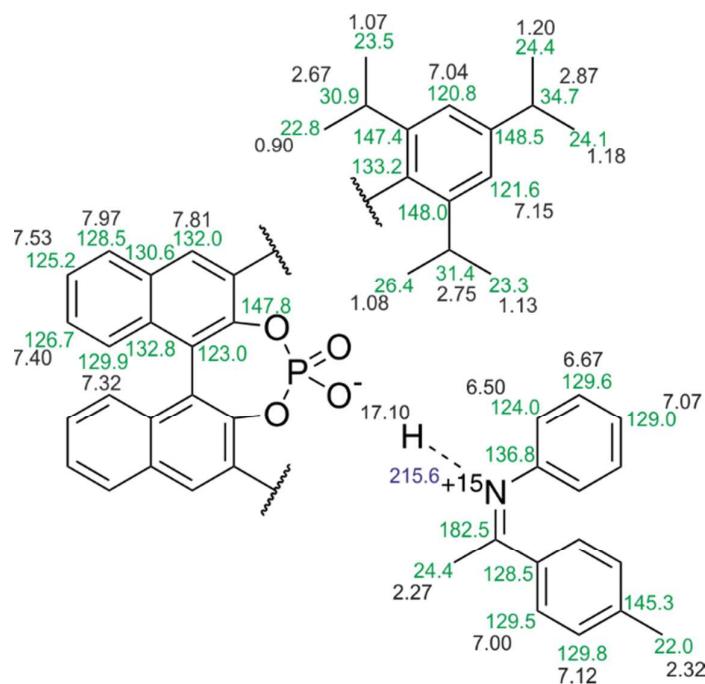
Complex 2b/1c

E-2b/1c
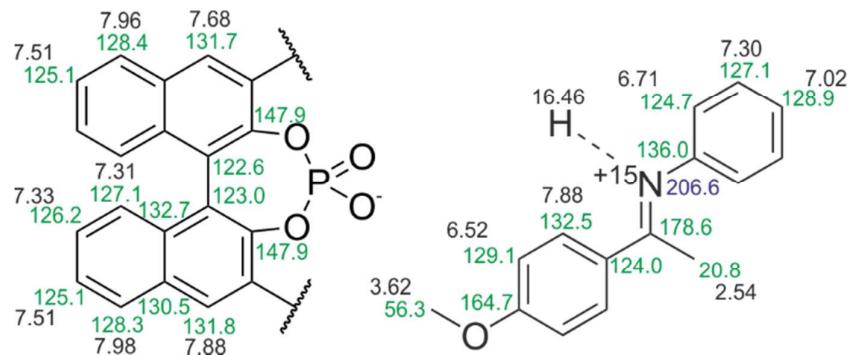
E-2b/1c
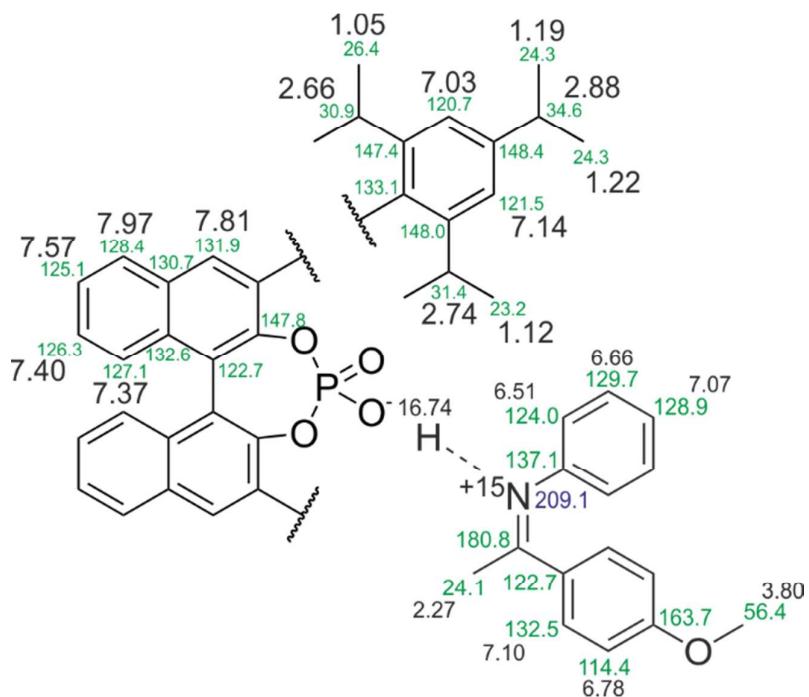
Complex 2c/1c

E-2c/1c
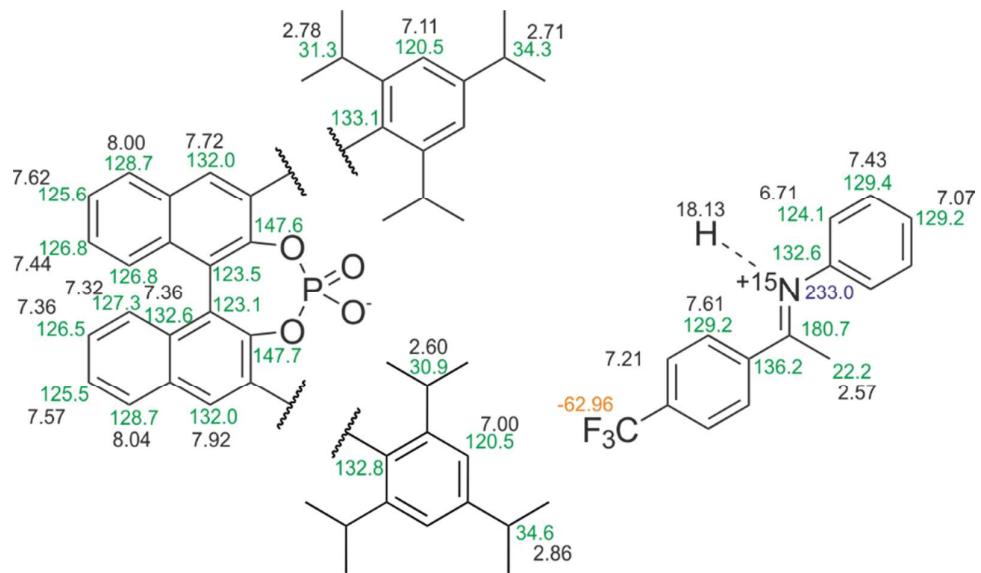
Z-2c/1c
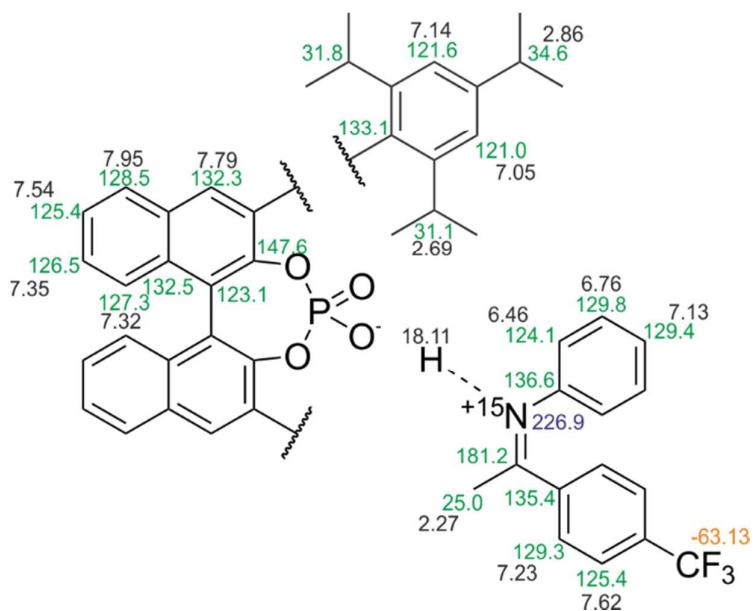
Complex 3a/1c

E-3a/1c
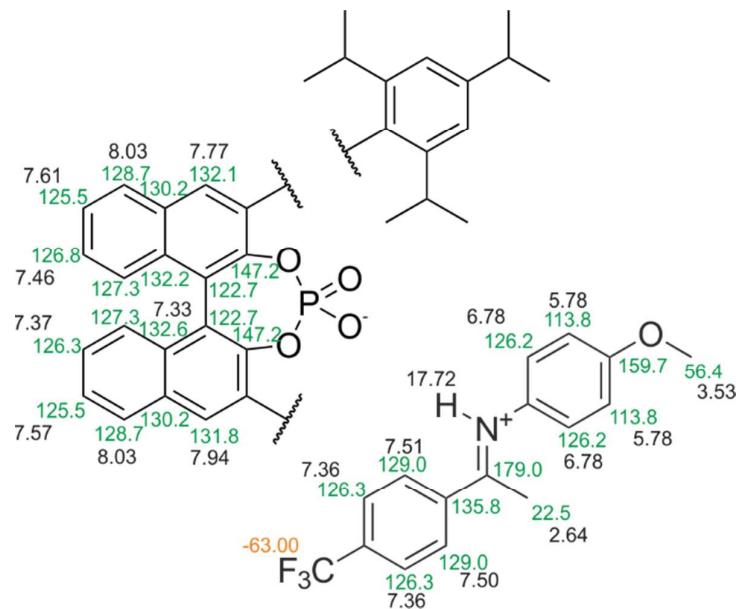
Z-3a/1c
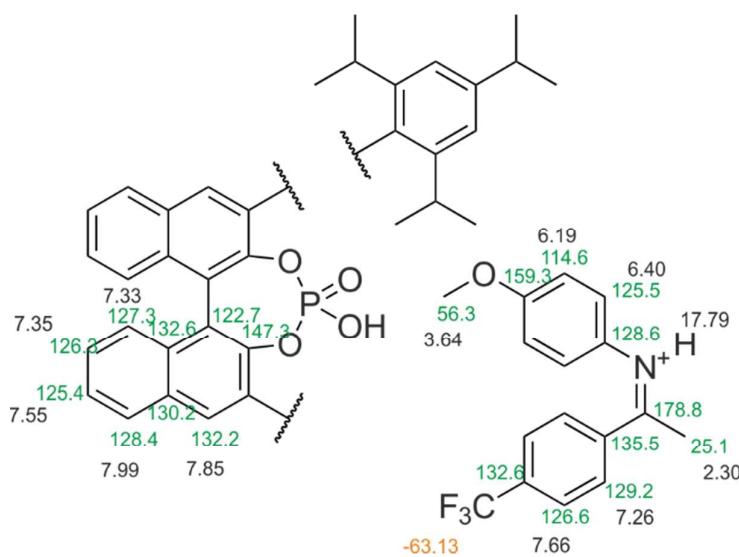
Complex 3b/1c

E-3b/1c
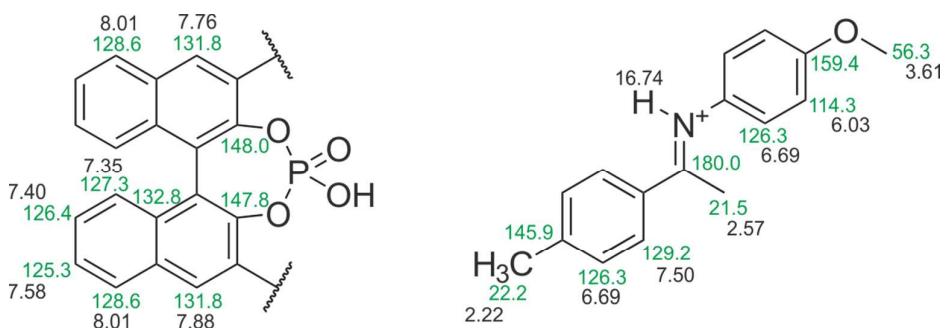
Z-3b/1c
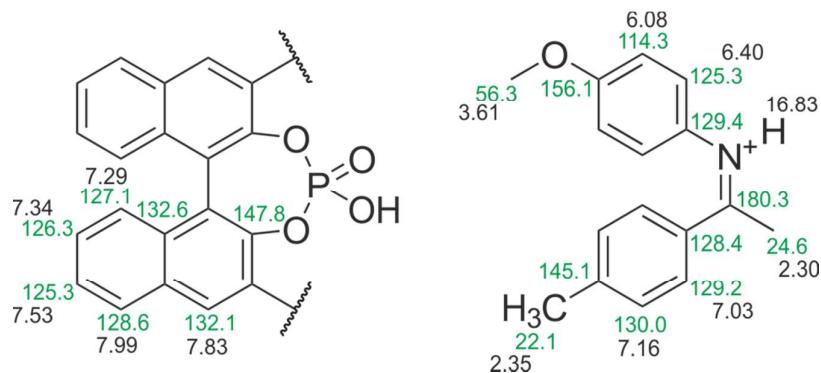
Low temperature measurements in the freonic solvent mixture

The NOE pattern for the investigated *Z*-imine/**1c** complexes showed that a fast exchange on the NMR time scale between two structures takes place, even at 180 K. Therefore we carried out measurements at as low as 130 K, in order to reach the slow exchange regime. For these measurements a freonic solvent mixture of CDF_2Cl and $CDFCl_2$ was used.
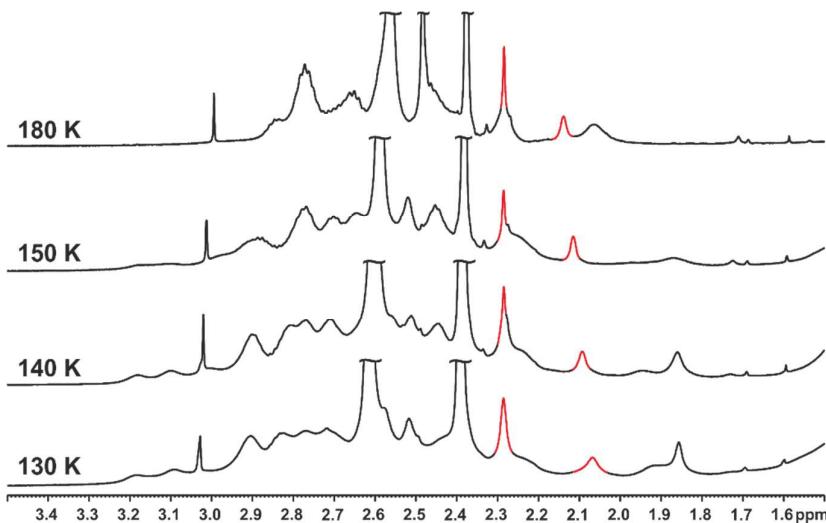
Figure S3: [1]H spectra of the **2a**/TRIP complex in a mixture of $CDFCl_2$ and CDF_2Cl at different temperatures. The signals labeled in red arise from the 4-methyl group and the methyl group of the imine. Compared to the other signal, no substantial line broadening was observed, even at 130 K.

By lowering the temperature, natural line broadening occurs. Even at 130 K, no substantial line broadening was observed for the *Z*-imine, when compared to the other signals.

Structure identification of all *E*-imine/TRIP complexes.

Selective ^{1}H NOESY spectra were used to identify the structures of complexes *E*-2a-b/1c in solution. For *E*-2c/1c and *E*-3a/1c, ^{1}H,[19]F HOESY spectra was used. The spectra were measured in CD_2Cl_2 at 180 K. In every investigated complex, the same orientations of the imine were observed. One orientation (*TYPE I E*)was identified by the NOE pattern between the varying functional groups on the ketone part of the imines and parts of the BINOL backbone of **1c**. In the complexes *E*-2a-b/1c, the functional groups, as well as signals of the BINOL backbone were excited in selective ^{1}H NOESY spectra. The other orientation (*TYPE II E*) was identified by 2D ^{1}H,[1]H NOESY spectra with a mixing time if 300 ms for imines **2a-c** and with selective 1D ^{1}H,[1]H NOESY spectra for imines **3a,b**. The methoxy group of the anisidine moiety of the imines was selectively excited in this case. In every investigated sample an exchange between the *E*-Isomer of the imine substrate inside the imine/**1c** complex and the free imine in solution was observed at 180 K. This chemical exchange leads to a variety of exchange peaks between the observed forms of the imine in the selective NOESY spectra. Additional signals are produced by spin diffusion effects inside the extended aromatic system. The exchange peaks and spin diffusion effects can be reduced by shortening the mixing time of the NOESY experiments, which also leads to a tremendous loss of signal intensity.

Additional 1D selective NOESY spectra where measured by exciting the ^{1}H signals of the BINOL backbone of the catalyst. Due to the large signal overlap in the aromatic region, these signals could not be excited selectively and therefor produced ambiguous NOEs. Nevertheless, these NOEs are in full agreement with the identified structure.

E-2a/1c complex

Structure of *TYPE I E*

Selective NOESY spectrum of complex *E*-2a/1c. The excited methyl group of imine **2a** is labeled yellow. Additional signals are observed, due to chemical exchange and spin diffusion effects.

Structure of *TYPE II E*
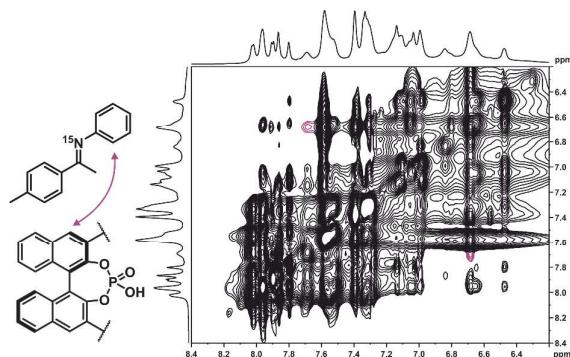
2D ^{1}H,^{1}H NOESY spectrum of complex **E-2a/1c**. The NOE that reveals structure **TYPE II E** is labeled in purple.

E-2b/1c complex

Structure of **TYPE I E**

Selective NOESY spectrum of complex **E-2b/1c**. The excited methoxy group of imine **2b** is labeled yellow. Additional signals are observed, due to chemical exchange and spin diffusion effects.

Structure of **TYPE II E**
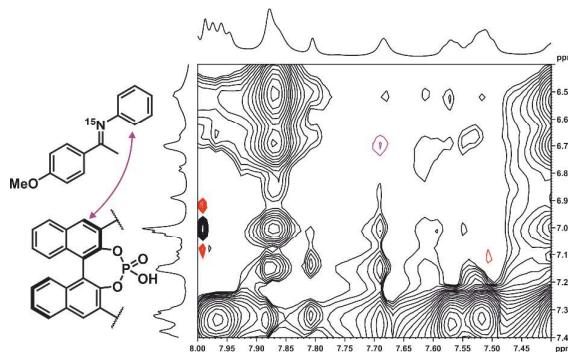
2D ^{1}H,^{1}H NOESY spectrum of complex **E-2b/1c**. The NOE that reveals structure **TYPE II E** is labeled in purple.

E-2c/1c complex

Structure of **TYPE I E**
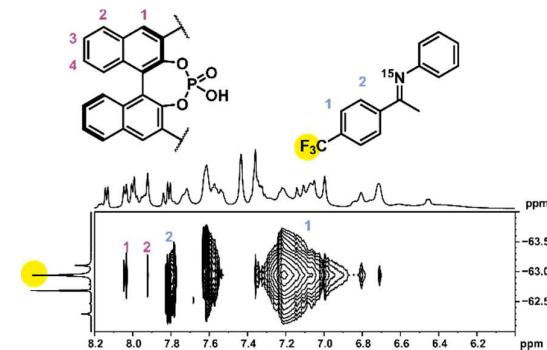
^{1}H,^{19}F HOESY spectrum of complex **E-2c/1c**. The trifluoromethyl group of **E-2c** inside the complex is labeled yellow. Additional signals are observed, due to chemical exchange and spin diffusion effects.

Structure of **TYPE II E**
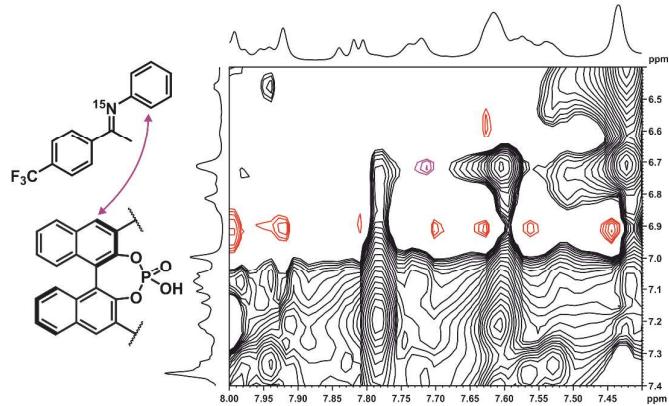
2D ^{1}H,^{1}H NOESY spectrum of complex **E-2c/1c**. The NOE that reveals structure **TYPE II E** is labeled in purple.

E-3a/1c complex

Structure of **TYPE I E**
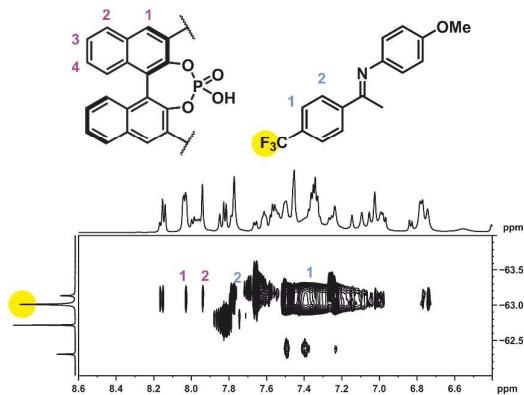
^{1}H,^{19}F HOESY spectrum of complex **E-3a/1c**. The trifluoromethyl group of **E-3a** inside the complex is labeled yellow. Additional signals are observed, due to chemical exchange and spin diffusion effects.

Structure of **TYPE II E**
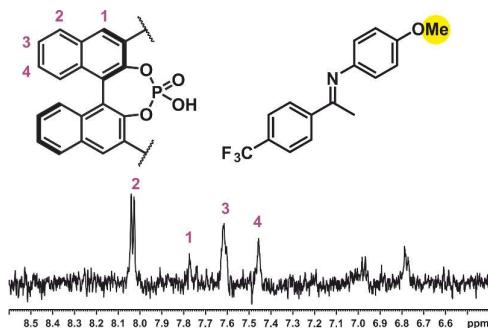
Selective NOESY spectrum of complex **E-3a/1c**. The excited methoxy group of imine **3a** is labeled yellow. Additional signals are observed, due to chemical exchange and spin diffusion effects.

E-3b/1c complex

Structure of *TYPE I E*
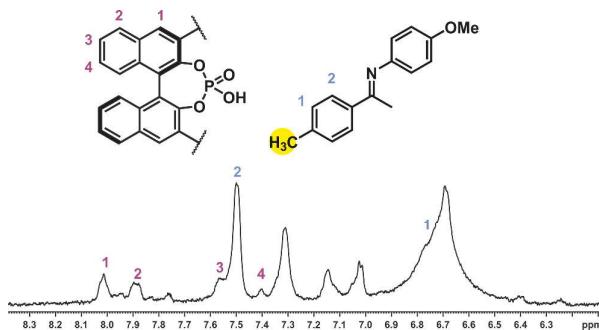
Selective NOESY spectrum of complex **E-3b/1c**. The excited methyl group of imine 3b is labeled yellow. Additional signals are observed, due to chemical exchange and spin diffusion effects.

## Structure of *TYPE II E*
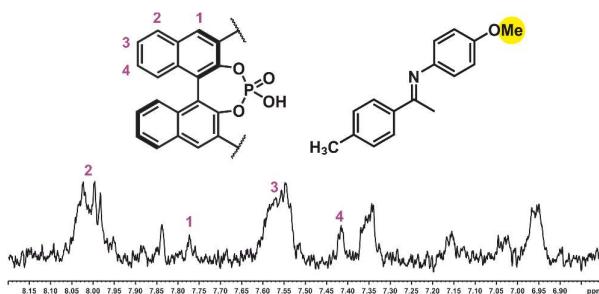
Selective NOESY spectrum of complex **E-3b/1c**. The excited methoxy group of imine **3b** is labeled yellow. Additional signals are observed, due to chemical exchange, chemical shift overlap and spin diffusion effects. Especially the overlap of the chemical shifts of the methoxy groups of both *E*- and *Z*-imine in complex **3b/1c** leads to many additional peaks in the selective NOESY.

Build-up curve
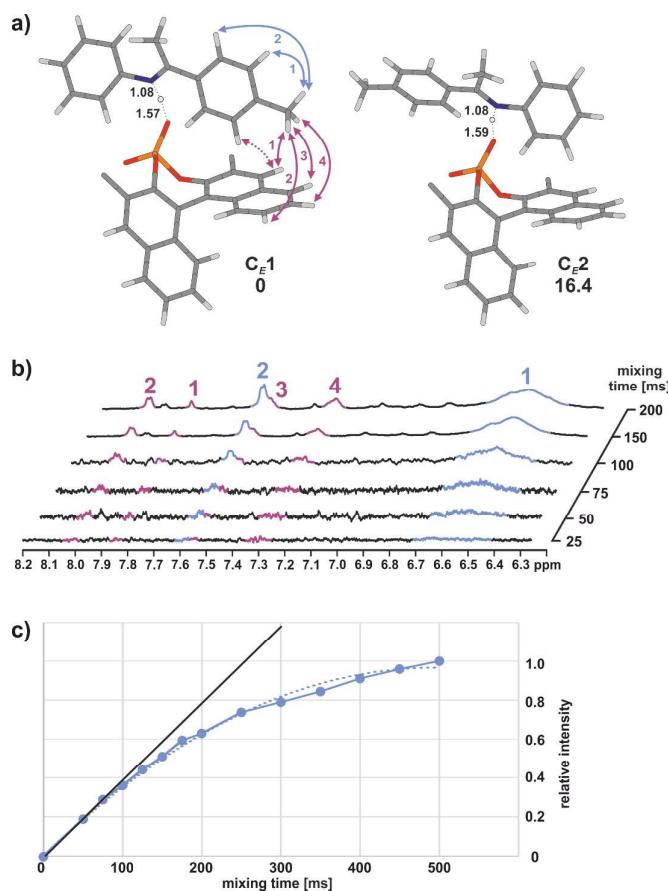
Figure S4; a) Complex structures *TYPE I E* and *TYPE II E* of complex *E-2a/1c*; b) Selective 1D NOESY build up curve; the α-methyl group of the imine was excited; c) Build-up of the intensity of intramolecular NOE 1 (blue arrow in a)), a deviation from a linear build is visible even at 100 ms mixing time, due to spin diffusion effects.

Structure identification of all *Z*-imine/TRIP complexes.

Selective ^{1}H NOESY spectra were used to identify the structures of complexes **Z-2a-c/1c** and **Z-3a/1c** in solution. In every investigated complex, the same NOE pattern was observed. The spectra were measured in CD_2Cl_2 at 180 K.

Z-2a/1c complex
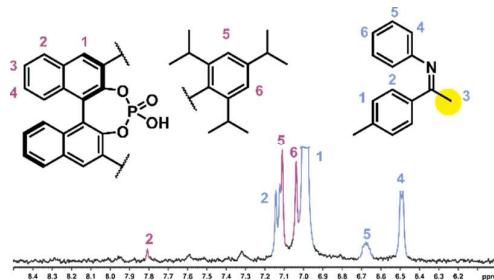
Selective NOESY spectrum of complex **Z-2a/1c**. The excited methyl group of imine **2a** is labeled yellow.

Z-2b/1c complex
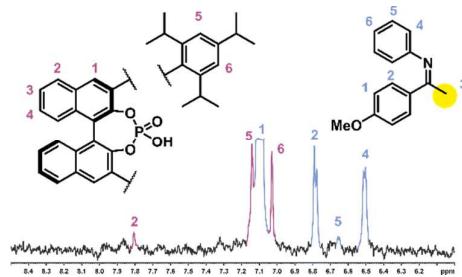
Selective NOESY spectrum of complex **Z-2b/1c**. The excited methyl group of imine **2b** is labeled yellow.

Z-2c/1c complex
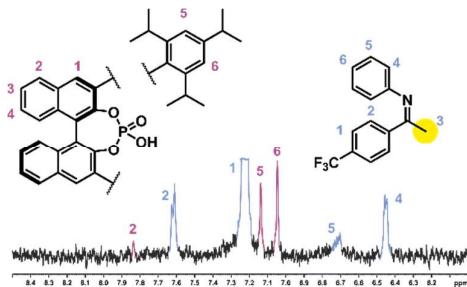
Selective NOESY spectrum of complex **Z-2c/1c**. The excited methyl group of imine **2c** is labeled yellow.

Z-3a/1c complex
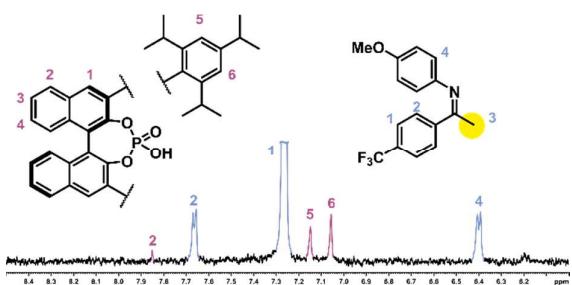
Selective NOESY spectrum of complex **Z-3a/1c**. The excited methyl group of imine **3a** is labeled yellow.

Z-3b/1c complex
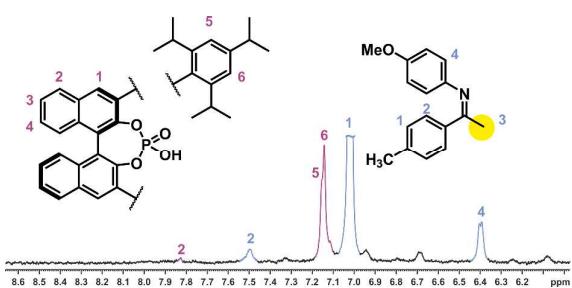
Selective NOESY spectrum of complex **Z-3b/1c**. The excited methyl group of imine **3b** is labeled yellow.

Chemical shift analysis of the 2a/1c complexes

The measured ^{1}H chemical shifts of the imine inside the complex are compared to the calculated chemical shifts.
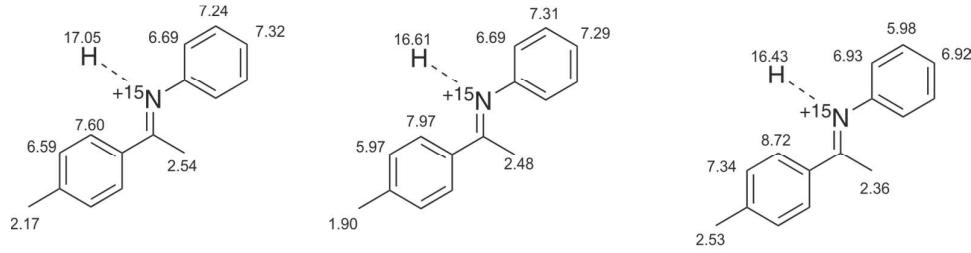
Measured   ***Type I E***   ***Type II E***

The calculated chemical shifts of complex ***TYPE I E*** show the same trend as the measured chemical shifts of the complex ***E-2a/1c*** in dichloromethane at 180 K. The strong high field shift of the *p*-methyl group and the nearby aromatic proton are a result of the strong deshielding due to the CH/π interaction of these protons and the BINOL backbone of the catalyst.
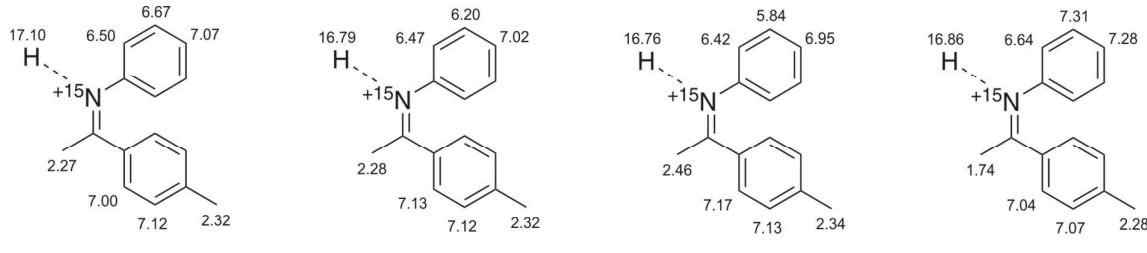
Measured   **Average**   ***Type I Z*** **75.8 %**   ***Type II Z*** **24.2 %**

The weighted and averaged chemical shifts of the calculated structures *TYPE II Z* and *TYPE I Z* are in good agreement with the measured shifts of complex ***E-2a/1c*** in dichloromethane at 180 K.

Spectrometer data

NMR experiments were performed on Bruker Avance III HD 400 MHz spectrometer, equipped with 5 mm BBO BB-1H/D probe head with Z-Gradients and a Bruker Avance III HD 600 MHz spectrometer, equipped with a 5 mm TBI 1H/19. Temperature was controlled in the VT-experiments by BVT 3000 and BVTE 3900. For NMR measurements employing standard NMR solvents 5 mm NMR tubes were used, if not other noted. For samples in freonic mixtures as solvents, 5 mm heavy wall (1.4 mm wall thickness) NMR tubes equipped with J. Young valves from Wilmad were used. NMR Data were processed, evaluated and plotted with TopSpin 3.2 software. Further plotting of the spectra was performed with Corel Draw X14 – X17 software. ^{1}H,^{13}C chemical shifts were referenced to TMS or the respective solvent signals. The heteronuclei ^{15}N,^{19}F and were referenced, employing $\nu(X) = \nu(TMS)$ x $\Xi_{reference}$ / 100 % according to Harris et al.[6] The following frequency ratios and reference compounds were used: $\Xi(^{15}N) = 10.132912$ (lq. NH_3) and $\Xi(^{19}F) = 94.094011$ (CCl_3F)

Pulse programs

All pulse programs used are standard Bruker NMR pulse programs.

Acquisition Parameters

^{1}H NMR: Pulse program: zg; Relaxation delay = 2 – 3 s, Acquisition time = 2.48 s, SW = 22.0 ppm, TD = 64k, NS = 8 – 64; zg30; Relaxation delay = 2 s, Acquisition time = 2.48 s, SW = 22.0 ppm, TD = 64k, NS = 8 – 64;

2D-^{1}H,^{1}H NOESY: Pulse program: noesygpph; Relaxation delay = 5 - 8 s, NS = 8-32, mixing time (D8) = 300.00 ms; TD = 4096; increments = 512 - 1k;

2D-^{1}H,^{1}H COSY: Pulse program: cosygpqf; Relaxation delay = 5 - 8 s, NS = 8-32, TD = 4096; increments = 512 - 1k;

^{13}C NMR: Pulse program: zgpg30; Relaxation delay = 2.00 s, Acquisition time = 0.80 s, SW = 270.0 ppm, TD = 64k, NS = 1k – 2k;

2D-^{1}H,^{13}C HSQC: Pulse program: hsqcedetgpsisp2.3; Relaxation delay = 4 - 8 s, NS = 8-32, $^1J_{XH}$ = 145 Hz; TD = 4096; increments = 512 - 1k;

2D-^{1}H,^{13}C HMBC: Pulse program: hmbcgplpndqf; Relaxation delay = 4 - 8 s, NS = 8-32, $^1J_{XH}$ = 145 Hz, J_{XH}(long range) = 10 Hz; TD = 4096; increments = 512 - 1k;

^{15}N NMR: Pulse program: zg; Relaxation delay = 10.00 s, Acquisition time = 0.54 s, SW = 502.8 ppm, TD = 32k, NS = 256 – 2048;

2D-^{1}H,^{15}N HMBC: Pulse program: inv4gplrndqf; Relaxation delay = 5 - 8 s, NS = 16-32, delay for evolution of long range couplings (D6) = 20.00 ms; TD = 4096; increments = 128 - 512;

^{19}F-NMR: Pulse program: zg30; Relaxation delay = 2 – 3 s, Acquisition time = 11.60 s, SW = 10.0 ppm, TD = 128k, NS = 8 – 64;

2D-^{1}H,^{19}F HOESY: Pulse program: hoesyph; Relaxation delay = 5 - 8 s, NS = 16-32, mixing time (D8) = 500.00 ms; TD = 4096; increments = 1k;

Selective 1D-^{1}H,^{1}H NOESY: Pulse program: selnogp; Relaxation delay = 5 - 8 s, NS = 128-2k, mixing time (D8) = 25 – 1000 ms (150 – 200 ms and NS = 1k-2k for structure identification); TD = 64k; 180° shaped pulse = 50 – 150 ms, shape = Gauss 180;

Data of the theoretical calculations

The CBS basis set extrapolation proceeds under the two point extrapolation procedure (eq.1 – 3) as in implemented in ORCA3.0.3[Neese, F. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2012**, *2*, 73.] with the basis set Def2-SVP and Def2-TZVP.

$$E_{\text{SCF}}^X = E_{\text{SCF}}^\infty + Ae^{-\alpha\sqrt{X}}$$

eq. 1

$$E_{\text{corr,MP2}}^\infty = \frac{X^\beta E_{\text{corr,MP2}}^X - (X-1)^\beta E_{\text{corr,MP2}}^{X-1}}{X^\beta - (X-1)^\beta}$$

eq.2

$$E_{\text{MP2}}^\infty = E_{\text{corr,MP2}}^\infty + E_{\text{SCF}}^\infty$$

eq. 3

Since low vibrations can cause significant error in the calculation of entropy, the harmonic approximation is corrected using the procedure by Grimme[Grimme, S. *Chem. - A Eur. J.* **2012**, *18*, 9955.], which employs a weighted partition function between harmonic and free rotor approximations.

NCI analysis
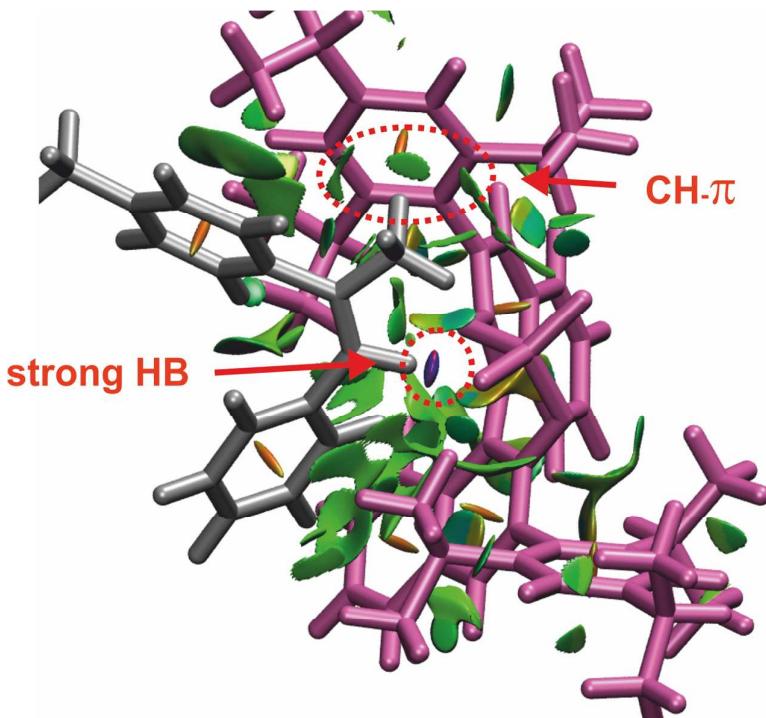
Figure S5. NCI analysis of Z-2a/1c *Type II*. Rotated view to highlight CH-π interaction between α-methyl group of the imine and 2,4,6-triisopropylphenyl group of the catalyst.

Table S1. Calculated energies of the (*R*)-TRIP imine complexes the solution phase

	Etot TPSS-D3	G180 TPSS-D3	Nimag	G180,solv. SCS-MP2
	Def2-SVP	Def2-SVP		CBS
me-ketimine/TRIP				
E-2a/1c conf0 (Type I)	-3216.1293034	-3214.9779909	0	-3210.8402178
E-2a/1c conf1 (Type I)	-3216.1292922	-3214.9783768	0	-3210.8405949
E-2a/1c conf2 (Type I)	-3216.1281091	-3214.9776036	0	-3210.8404332
E-2a/1c conf0 (Type II)	-3216.1288254	-3214.9770885	0	-3210.8379438
E-2a/1c conf1 (Type II)	-3216.1288923	-3214.9771949	0	-3210.8380750
E-2a/1c conf2 (Type II)	-3216.1281937	-3214.9763154	0	-3210.8371123
Z-2a/1c conf0 (Type II)	-3216.1239436	-3214.9742384	0	-3210.8370365
Z-2a/1c conf1 (Type II)	-3216.1239479	-3214.9737243	0	-3210.8365321
Z-2a/1c conf2 (Type II)	-3216.1230459	-3214.9719391	0	-3210.8358809
Z-2a/1c conf3 (Type II)	-3216.1243248	-3214.9733132	0	-3210.8352594
Z-2a/1c conf0 (Type I)	-3216.1216601	-3214.9718608	0	-3210.8346718
Z-2a/1c conf1 (Type I)	-3216.1216456	-3214.9716979	0	-3210.8346181
Z-2a/1c conf2 (Type I)	-3216.1212309	-3214.9701984	0	-3210.8321087
ome-ketimine/TRIP				
E-2b/1c conf0 (Type I)	-3291.2958062	-3290.143671	0	-3285.9698539
E-2b/1c conf1 (Type I)	-3291.2957223	-3290.143170	0	-3285.9693529
E-2b/1c conf2 (Type I)	-3291.2947169	-3290.142961	0	-3285.9689460
E-2b/1c conf0 (Type II)	-3291.2952666	-3290.143039	0	-3285.9678192
E-2b/1c conf1 (Type II)	-3291.2940632	-3290.142076	0	-3285.9676053
E-2b/1c conf2 (Type II)	-3291.2955281	-3290.141910	0	-3285.9676420
E-2b/1c conf3 (Type II)	-3291.2942653	-3290.141420	0	-3285.9668046
E-2b/1c conf4 (Type II)	-3291.2942222	-3290.141566	0	-3285.9673435
E-2b/1c conf5 (Type II)	-3291.2953907	-3290.142301	0	-3285.9680170
Z-2b/1c conf0 (Type II)	-3291.2881317	-3290.138687	0	-3285.9654871
Z-2b/1c conf1 (Type II)	-3291.2880073	-3290.138259	0	-3285.9657424
Z-2b/1c conf2 (Type II)	-3291.2873514	-3290.136991	0	-3285.9656882
Z-2b/1c conf3 (Type II)	-3291.2887209	-3290.139127	0	-3285.9655835
Z-2b/1c conf4 (Type II)	-3291.2881877	-3290.137369	0	-3285.9655633
Z-2b/1c conf5 (Type II)	-3291.2881191	-3290.138095	0	-3285.9654841
Z-2b/1c conf6 (Type II)	-3291.2873533	-3290.136156	0	-3285.9647129
Z-2b/1c conf7 (Type II)	-3291.2887316	-3290.138912	0	-3285.9650782
Z-2b/1c conf0 (Type I)	-3291.2861415	-3290.135660	0	-3285.9628199
Z-2b/1c conf1 (Type I)	-3291.2861924	-3290.135523	0	-3285.9628561
Z-2b/1c conf2 (Type I)	-3291.2858786	-3290.134948	0	-3285.9615452
Z-2b/1c conf3 (Type I)	-3291.2863205	-3290.137066	0	-3285.9639722
Z-2b/1c conf4 (Type I)	-3291.2864156	-3290.136289	0	-3285.9632361
Z-2b/1c conf5 (Type I)	-3291.2860152	-3290.137701	0	-3285.9634013
cf3-ketimine/TRIP				
E-2c/1c conf0 (Type I)	-3513.6465830	-3512.5205064	0	-3508.3958759
E-2c/1c conf1 (Type I)	-3513.6465235	-3512.5207007	0	-3508.3960729
E-2c/1c conf2 (Type I)	-3513.6457328	-3512.5204823	0	-3508.3959762

E-2c/1c conf0 (Type II)	-3513.6375353	-3512.5171876	0	-3508.3919597
E-2c/1c conf1 (Type II)	-3513.6375690	-3512.5187441	0	-3508.3936257
E-2c/1c conf2 (Type II)	-3513.6372055	-3512.5172824	0	-3508.3923135
Z-2c/1c conf0 (Type II)	-3513.6411194	-3512.5141016	0	-3508.3916784
Z-2c/1c conf1 (Type II)	-3513.6411936	-3512.5140964	0	-3508.3917285
Z-2c/1c conf2 (Type II)	-3513.6399301	-3512.5135202	0	-3508.3919537
Z-2c/1c conf3 (Type II)	-3513.6416873	-3512.5142537	0	-3508.3903968
Z-2c/1c conf0 (Type I)	-3513.6375353	-3512.5110397	0	-3508.3897986
Z-2c/1c conf1 (Type I)	-3513.6375690	-3512.5114201	0	-3508.3900476
Z-2c/1c conf2 (Type I)	-3513.6372055	-3512.5104673	0	-3508.3876702
ome-cf3-ketimine/TRIP				
E-3a/1c conf0 (Type I)	-3628.111866	-3626.9518503	0	-3622.7355951
E-3a/1c conf1 (Type I)	-3628.111719	-3626.9517008	0	-3622.7359474
E-3a/1c conf2 (Type I)	-3628.110813	-3626.9529548	0	-3622.7367638
E-3a/1c conf3 (Type I)	-3628.112400	-3626.9534522	0	-3622.7374813
E-3a/1c conf4 (Type I)	-3628.112112	-3626.9539513	0	-3622.7383783
E-3a/1c conf5 (Type I)	-3628.111580	-3626.9526340	0	-3622.7359897
E-3a/1c conf0 (Type II)	-3628.111930	-3626.9529648	0	-3622.7347878
E-3a/1c conf1 (Type II)	-3628.112139	-3626.9524390	0	-3622.7341516
E-3a/1c conf2 (Type II)	-3628.111372	-3626.9519985	0	-3622.7342329
Z-3a/1c conf0 (Type II)	-3628.106399	-3626.9475052	0	-3622.7332675
Z-3a/1c conf1 (Type II)	-3628.106393	-3626.9473794	0	-3622.7330704
Z-3a/1c conf2 (Type II)	-3628.104956	-3626.9463497	0	-3622.7331959
Z-3a/1c conf3 (Type II)	-3628.107676	-3626.9492683	0	-3622.7338728
Z-3a/1c conf0 (Type I)	-3628.101010	-3626.9434394	0	-3622.7305094
Z-3a/1c conf1 (Type I)	-3628.101616	-3626.9416407	0	-3622.7262811
Z-3a/1c conf2 (Type I)	-3628.101561	-3626.9436228	0	-3622.7309610
Z-3a/1c conf3 (Type I)	-3628.101626	-3626.9438736	0	-3622.7311135
Z-3a/1c conf4 (Type I)	-3628.101963	-3626.9422244	0	-3622.7264107
ome-ch3-ketimine/TRIP				
E-3b/1c conf0 (Type I)	-3330.592144	-3329.4088051	0	-3325.1805363
E-3b/1c conf1 (Type I)	-3330.592006	-3329.4089581	0	-3325.1810063
E-3b/1c conf2 (Type I)	-3330.591542	-3329.4093499	0	-3325.1804439
E-3b/1c conf3 (Type I)	-3330.593070	-3329.4106280	0	-3325.1822841
E-3b/1c conf4 (Type I)	-3330.592881	-3329.4105133	0	-3325.1823263
E-3b/1c conf0 (Type II)	-3330.594000	-3329.4103556	0	-3325.1787176
E-3b/1c conf1 (Type II)	-3330.593958	-3329.4105325	0	-3325.1790970
E-3b/1c conf2 (Type II)	-3330.593524	-3329.4096527	0	-3325.1785529
Z-3b/1c conf0 (Type II)	-3330.588810	-3329.4073733	0	-3325.1791460
Z-3b/1c conf1 (Type II)	-3330.588676	-3329.4071171	0	-3325.1788328
Z-3b/1c conf2 (Type II)	-3330.587739	-3329.4052449	0	-3325.1780921

Z-3b/1c conf3 (Type II)	-3330.589223	-3329.4070524	0	-3325.1776291
Z-3b/1c conf0 (Type I)	-3330.584634	-3329.4032057	0	-3325.1753078
Z-3b/1c conf1 (Type I)	-3330.584538	-3329.4035100	0	-3325.1754672
Z-3b/1c conf2 (Type I)	-3330.584521	-3329.4023288	0	-3325.1726030
Z-3b/1c conf3 (Type I)	-3330.585319	-3329.4033326	0	-3325.1751190
Z-3b/1c conf4 (Type I)	-3330.585216	-3329.4032161	0	-3325.1751941
Z-3b/1c conf5 (Type I)	-3330.584905	-3329.4038217	0	-3325.1740197
ome-no2-ketimine/TRIP				
E-3c/1c conf0 (Type I)	-3495.681803	-3494.5237310	0	-3490.2561506
E-3c/1c conf1 (Type I)	-3495.681937	-3494.5233009	0	-3490.2559409
E-3c/1c conf2 (Type I)	-3495.681214	-3494.5223690	0	-3490.2543048
E-3c/1c conf0 (Type II)	-3495.683907	-3494.5256113	0	-3490.2545437
E-3c/1c conf1 (Type II)	-3495.683703	-3494.5247775	0	-3490.2537381
E-3c/1c conf2 (Type II)	-3495.682741	-3494.5247566	0	-3490.2541695

Optimized geometry

Solution Phase 2a/1c

E-configuration

E-2a/1c (Type I; conf0)
1\1\GINC-LOGIN\FOpt\RTPSSTPSS\def2SVP/W06\C65H72N1O4P1\JHIOE\20-Dec-20
14\0\\#p opt tpsstpss/def2svp/w06 densityfit empiricaldispersion=gd3 s
crf=(smd,solvent=ch2cl2,read)\\title\\0,1\P,-0.1126479016,-0.462480476
1,-1.2372328786\O,-1.4272845126,0.5640547744,-1.3980511967\O,0.8329740
653,0.4683672862,-0.1759706766\O,0.4925398423,-0.579455675,-2.60446895
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441,0.2849235484\C,-1.9802225745,1.1911739916,-0.3021237546\C,-3.27900
53629,0.7652044112,0.1215294585\C,-3.8632487064,1.4306859834,1.1912956
121\H,-4.8654470709,1.1403220866,1.5236087856\C,-3.1794381872,2.460319
3149,1.8987137342\C,-1.8678452328,2.8726159221,1.4616304382\C,-1.16580
30596,3.8331085673,2.2513769499\H,-0.1509359621,4.1214978914,1.9633407
957\C,-1.7406566961,4.3854641325,3.3867555149\H,-1.1764069414,5.112503
6254,3.9811313871\C,-3.0503445598,4.0100576973,3.789961075\H,-3.495753
0069,4.4580885616,4.6848582146\C,-3.7508185411,3.0626338886,3.06007052
78\H,-4.7516023564,2.7449732693,3.3741196122\C,0.0041600272,2.71773166
22,-0.2784130069\C,1.0516805112,1.804567912,-0.43741567\C,2.3859762201
,2.2014104895,-0.7646805258\C,2.6188795203,3.5417625231,-1.0386748252\
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,2.8164322218,6.1582119207,-1.6774651053\C,-1.4787912512,-0.6230495263
,4.6703048052\C,-0.9842584849,-1.8486316053,5.1641037931\H,-1.34843961
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88\H,-1.3313009653,0.7981605827,3.0329618641\C,1.391292986,-2.93422824
61,2.4234025086\C,2.4078200629,-3.7650264896,3.147131138\H,3.307110898
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\H,2.6852236125,-3.2727288984,4.0914908541\N,1.3603843166,-2.864731736
6,1.1106474154\H,0.5966009657,-2.2793030688,0.6177126406\C,2.195279040
3,-3.5366619731,0.1626507928\C,2.7062769888,-2.7744903347,-0.904577558
\H,2.5304626853,-1.6966747872,-0.9481455078\C,3.4666636294,-3.40514651
21,-1.8966604699\H,3.8707657722,-2.8068941053,-2.7183433481\C,3.717116
7681,-4.7845057218,-1.8301770229\C,3.1973342092,-5.5394026846,-0.76671
67176\H,3.3771312911,-6.6183848007,-0.7163149783\C,2.4277835221,-4.923
4646208,0.2295711059\H,1.9851846728,-5.5190874853,1.0321162256\C,3.493
1334531,1.1911966272,-0.7298291995\C,4.0605510704,0.6941047798,-1.9309
169709\C,3.971291968,0.7320011001,0.530795681\C,5.1143656523,-0.237836
3729,-1.8464105835\C,5.0161066681,-0.2062909212,0.5598007445\C,5.60179
25028,-0.7080434652,-0.6172484641\H,5.5585000732,-0.6248464954,-2.7710
76375\H,5.3836438905,-0.5584146989,1.5284863816\C,-3.980729902,-0.3533
782816,-0.5849773558\C,-4.2243526646,-1.5824854122,0.0867695686\C,-4.4
244573083,-0.1797452766,-1.9264852619\C,-4.925322805,-2.5992786975,-0.
5909342362\C,-5.1173387455,-1.2270487521,-2.5574443332\C,-5.3832422205
,-2.4461627431,-1.908491333\H,-5.1157148042,-3.5484662616,-0.075115651
2\H,-5.4661077289,-1.0821310588,-3.5868018729\H,4.3127554314,-5.272008
6627,-2.60904075\C,-2.5150121768,0.17435047,5.4212314966\H,-3.46095626
54,0.2067497154,4.8484297689\H,-2.7260807541,-0.2602185816,6.412061831
9\H,-2.1884746288,1.2211959857,5.555088898\C,-4.2054300642,1.124778503
9,-2.6960033157\H,-3.6229200012,1.8074854376,-2.0552102307\C,-3.729333
0305,-1.8521009005,1.5096013992\C,-6.1495392434,-3.5654714985,-2.60798
69461\H,-6.180282904,-4.4221355221,-1.9084362414\C,-4.8995336648,-1.92
37153689,2.5123226603\H,-4.5232178389,-2.095969749,3.5376181705\H,-5.4
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9\H,-5.9746191856,-4.8881134483,-4.3461266652\C,-7.6054613206,-3.14841
13001,-2.9032035996\H,-8.1679930748,-3.9853284835,-3.3566575958\H,-8.1
290945732,-2.8436339536,-1.9793958819\H,-7.6399158359,-2.2977254808,-3
.6088832948\C,-3.3866145328,0.8994681785,-3.9832856098\H,-3.9302500359
,0.2598761811,-4.7031500795\H,-3.1828697935,1.8651852884,-4.4819030711
\H,-2.4200674411,0.4215656477,-3.751306876\C,-5.5475159952,1.825363138
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,-0.2406017208\H,8.911859254,-1.7589834072,-0.2461996473\H,8.311707245
9,-0.239584925,-0.9772850645\H,8.0452823711,-0.5606226828,0.7603004542
\C,6.4660487171,-2.8797246177,0.413544208\H,6.4435994463,-2.5269805493
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369132372\H,2.8602832432,0.6764714473,3.8593813029\C,4.1106830949,2.60
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55,-3.2669100021\H,5.5345151832,1.7072002595,-4.0980568045\H,4.1651257
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554,-4.5051330812\H,2.5602015033,-0.7140823466,-3.823689189\C,-2.85693
90459,-3.1216766925,1.5813784034\H,-3.4437356077,-4.0342434959,1.36786
09774\H,-2.0285240431,-3.0559874747,0.8572400539\H,-2.427913914,-3.230
197435,2.5940726036\H,-3.0872889763,-1.0074751155,1.8073858934\\Versio
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3e-06\Dipole=1.7071068,-2.3988167,5.0282876\Quadrupole=-8.3754467,12.7
911566,-4.4157099,-17.1936985,-4.8680905,-13.7482685\PG=C01 [X(C65H72N
1O4P1)]\\@

E-2a/1c (Type I; conf1)
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crf=(smd,solvent=ch2cl2,read)\\title\\0,1\P,-0.1011446316,-0.381696061
9,-1.3053979587\O,-1.3822205925,0.6833982565,-1.4840537197\O,0.8261569
238,0.4942645244,-0.1829509614\O,0.5563266402,-0.4716094397,-2.6505793
637\O,-0.5213671571,-1.5974615169,-0.4855823064\C,-1.2551259372,2.3460
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17405104,0.8936664028,-0.0005778465\C,-3.8595223409,1.5585199933,1.061
9581279\H,-4.8753214905,1.2848511886,1.3655159574\C,-3.1739990527,2.56
69865261,1.797837331\C,-1.8420301097,2.954865256,1.4019800193\C,-1.142
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31962\C,-1.7376376598,4.4468599707,3.344949566\H,-1.175092692,5.156129
2462,3.9620101474\C,-3.0664190836,4.0972562364,3.7065411205\H,-3.52790
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429,-0.2831085757\C,1.100635401,1.8250850793,-0.416500735\C,2.45779191
47,2.1792157103,-0.6940301957\C,2.7422028406,3.5128623136,-0.952248756
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\C,-0.3327534006,6.4486454497,-1.0650711833\H,-1.1268808491,7.20144178
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S30

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297,-2.7238786999\C,-2.6052179959,0.1681538305,5.335065329\H,-3.508443
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62582,-1.7416229063,1.3351139161\C,-6.1477767541,-3.3699028853,-2.8177
703254\H,-6.4123095491,-2.9752442266,-3.816995764\C,-4.8741328141,-1.7
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\H,-8.0315373383,-4.4812335604,-2.668024392\C,-5.2703783565,-4.6216812
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149105375,2.1021871234,-3.7673203357\H,4.8602209136,2.9651761708,-3.09
38790327\H,5.6988094913,1.6180848551,-3.9126300714\H,4.3764001354,2.48
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3847615549\H,2.666013465,-0.7363977543,-3.7713690267\C,-2.9158691077,-
3.0572986217,1.4067142372\H,-3.5553232496,-3.9385314006,1.2137756621\H
,-2.0963120255,-3.0455863227,0.6699851393\H,-2.4785703589,-3.179243202
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E-2a/1c (Type I; conf2)
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688392\C,-1.8128274372,4.6671981046,2.9859029649\H,-1.2673871841,5.403
9821715,3.5858463983\C,-3.1695109561,4.3755854361,3.2907139562\H,-3.66
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3828638639\H,-1.5665349771,1.1039749373,2.9119190745\C,0.9226474933,-2
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,-0.2029140833,-0.8967287373\C,-4.2425633086,-1.3968183427,-0.18757717
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H,-3.8523852892,0.7897225959,4.5421029066\H,-3.3334141682,0.302087588,
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,1.1812877432,-3.0771829641\H,-3.4181959149,1.8754912235,-2.426730909\
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,-2.9216667181\H,-6.199041163,-3.1301281895,-3.9643023668\C,-5.0573096
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108044567\C,7.0460374087,-1.6460791638,0.0359668846\H,7.2414101257,-1.
6770685537,1.1245929312\C,3.8276826884,0.7935674175,-3.0736642026\H,2.
8437018021,1.2874845027,-3.0000915047\C,3.2921067867,1.1494704644,2.03
20695803\H,2.244892699,1.3493719544,1.7480555666\C,6.7958763383,-3.094
4008396,-0.4307129855\H,7.6847569127,-3.7231428518,-0.2382643122\H,5.9
379875657,-3.5419533173,0.100092452\H,6.5831030595,-3.1325587823,-1.51
47268695\C,8.2952311346,-1.0519064096,-0.6455117936\H,8.1778234825,-1.
0243885136,-1.7443629088\H,8.4880415412,-0.020818221,-0.2986955325\H,9
.1886930631,-1.6624729884,-0.4197723981\C,3.2547104503,0.1573940422,3.
2080309061\H,2.8897732262,-0.8327194261,2.8853159913\H,4.2513204727,0.
020847958,3.6658367478\H,2.5789013883,0.5323333279,3.9969683557\C,3.91
5985217,2.4926821044,2.4687069386\H,3.8891881812,3.2312216927,1.648588
9312\H,3.3656860957,2.9158324172,3.3292710999\H,4.970974315,2.35332892
56,2.7689643864\C,4.8111786757,1.780438928,-3.7369071596\H,4.912872197
9,2.7084280509,-3.1470661714\H,5.8168832131,1.3304762482,-3.8344619808
\H,4.4628060808,2.0561342056,-4.7494013493\C,3.6307431697,-0.463565517
6,-3.9433325229\H,3.255743588,-0.1750515923,-4.942594271\H,4.577622586
2,-1.0141212199,-4.0924571608\H,2.8863193815,-1.1344228953,-3.48514723
92\C,-3.0873290834,-2.9324631439,1.4885074309\H,-3.7416297116,-3.80717
44119,1.3173112868\H,-2.2218836374,-2.9984902929,0.8090768244\H,-2.718
6654512,-2.9937493859,2.5284933069\H,-3.1421601782,-0.7937569529,1.542
1042462\\Version=ES64L-G09RevD.01\State=1-A\HF=-3216.1281091\RMSD=5.46
5e-09\RMSF=2.648e-06\Dipole=1.0586791,-2.1603543,5.3634226\Quadrupole=
-9.2668891,12.0313059,-2.7644168,-13.8670923,-5.8524785,-15.7736362\PG
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E-2a/1c (Type II; conf0)
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15\0\\#p tpsstpss/def2svp/w06 densityfit empiricaldispersion=gd3 opt s
crf=(smd,solvent=ch2cl2,read)\\title\\0,1\P,-0.2953986811,-0.688130029
4,-0.9302185863\O,-1.6018888406,0.2874744117,-1.3143601289\O,0.6930495
261,0.4542612082,-0.1579349648\O,0.2594490128,-1.1782931261,-2.2337877
527\O,-0.6657889326,-1.6249329102,0.2208221121\C,-1.4820970387,2.24418
26293,0.0503291888\C,-2.1561965746,1.0829116291,-0.3332797708\C,-3.435
32709,0.7085286887,0.1844875998\C,-4.0039787045,1.5295318785,1.1489081
417\H,-4.995094822,1.2890188414,1.5467128656\C,-3.3183544237,2.6656421
827,1.6667890555\C,-2.0289359098,3.0266302485,1.1305441613\C,-1.327846
704,4.1159732678,1.7308756597\H,-0.3308103668,4.3763687041,1.362866645
5\C,-1.8813227194,4.8278048984,2.785564092\H,-1.3189792332,5.651530074
6,3.238876558\C,-3.1673969086,4.492951287,3.2885940982\H,-3.5952172355
,5.0660916268,4.1183471088\C,-3.8682962725,3.431221167,2.7383781825\H,
-4.8513534696,3.1478842377,3.1311289264\C,-0.2167944251,2.6225589485,-
0.6416105747\C,0.8493991498,1.7176714266,-0.6908368825\C,2.1464733365,
2.0800822962,-1.1736313432\C,2.3146457288,3.3498513133,-1.7079353154\H
,3.306333867,3.6608696071,-2.0529253527\C,1.2297812912,4.2677089415,-1
.8168042786\C,-0.0586750488,3.9064599296,-1.2785038757\C,-1.1362462891
,4.8315978909,-1.4282335775\H,-2.1282292119,4.5600306426,-1.0558454281
\C,-0.9470423664,6.0556274202,-2.0530367506\H,-1.7917181427,6.74449424
73,-2.1643356523\C,0.3301675654,6.4207933869,-2.5568047837\H,0.4670479
734,7.3923401763,-3.0441019298\C,1.3942540245,5.540089756,-2.442332586

2\H,2.3811260906,5.8032220262,-2.8400477517\C,3.9277841498,-4.46662501
82,-0.738169701\C,4.6042785124,-4.2340883963,0.4762758215\H,5.64205054
42,-4.5651083937,0.5889858142\C,3.9824377372,-3.5702481284,1.536357167
6\H,4.5547716353,-3.4040684443,2.4519280599\C,2.647205994,-3.107022389
,1.4238918123\C,1.9524744662,-3.3831317826,0.2165941458\H,0.9119638746
,-3.0729360665,0.088361921\C,2.5838548003,-4.0397362309,-0.8363392117\
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,2.8431189956,-3.1645644182,4.3632569114\N,0.827733576,-1.8411916239,2
.3939111322\H,0.330487947,-1.8202101875,1.4394499349\C,0.052231336,-1.
1720800112,3.3928465147\C,-0.5068857016,0.0774120324,3.0654216138\H,-0
.3160580942,0.515517004,2.0821876676\C,-1.3016146711,0.7407182396,4.00
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5506103,5.2593614445\C,-1.018393525,-1.1044042824,5.567054286\H,-1.231
017002,-1.5755903593,6.5324334258\C,-0.2135223956,-1.7747580861,4.6364
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3752,-0.5816577309\H,5.1907600978,-1.2148575758,-2.5845023177\H,5.6559
402106,0.3836606552,1.3906252431\C,-4.1356353286,-0.5132947242,-0.3254
558956\C,-4.342123228,-1.6309149124,0.52920607\C,-4.6159568176,-0.5472
578054,-1.6651788268\C,-5.0617108349,-2.7369029115,0.0362047795\C,-5.3
159428535,-1.6815894879,-2.1109452732\C,-5.5609235183,-2.785156778,-1.
2748237529\H,-5.230467779,-3.5983791691,0.6937424736\H,-5.6861821653,-
1.7005286229,-3.1427807995\H,-2.1867972214,0.6758780333,5.9892003207\C
,4.6099180282,-5.1226303078,-1.9098218727\H,4.6926501515,-4.4059631329
,-2.7489103675\H,5.6229668677,-5.4711817651,-1.6511832536\H,4.02150671
61,-5.9814176564,-2.280730091\C,-4.4224581264,0.6218417879,-2.63324669
38\H,-3.8389092044,1.4014215742,-2.116113424\C,-3.7901846774,-1.680893
6092,1.9559301066\C,-6.3213485488,-4.0081420622,-1.77930585\H,-6.42409
80743,-4.7015140074,-0.923404321\C,-4.9080593861,-1.4984121263,3.00328
40436\H,-4.4861161943,-1.4943785736,4.0252655307\H,-5.4511154088,-0.54
88151523,2.8550577743\H,-5.6459396537,-2.3204824845,2.9448481424\C,-5.
5307781882,-4.7429363228,-2.8820441285\H,-5.402203024,-4.1023123807,-3
.7739846125\H,-5.5260631979,-5.0319446517,-2.5252833941\H,-6.061295242
4,-5.6603257203,-3.1972379615\C,-7.7410148687,-3.645341838,-2.26087623
78\H,-8.2919555994,-4.5534334428,-2.5673115042\H,-8.3185879593,-3.1471
797743,-1.4615816587\H,-7.7077268014,-2.9632291772,-3.1303033906\C,-3.
6182139275,0.2006653222,-3.8801264321\H,-4.1653361057,-0.5505281524,-4
.4794554542\H,-3.4317627406,1.0756211031,-4.5299997355\H,-2.6434684279
,-0.2254373002,-3.5890901288\C,-5.7744110753,1.2565462521,-3.020145223
3\H,-5.6162188245,2.1391953152,-3.6668600805\H,-6.4125392699,0.5434258
493,-3.5741294827\H,-6.3309217843,1.5843846753,-2.1235664039\C,6.83226
14309,-1.3747954796,-0.4425700299\H,6.5886971656,-2.3576215788,-0.8909
900334\C,3.005044956,0.2398743592,-3.3599699745\H,1.967673219,0.567201
9793,-3.1718651278\C,3.5541271675,2.0839703039,1.4080653661\H,2.644184
4927,2.6162293367,1.0831039039\C,7.9911347044,-0.7694067889,-1.2672060
571\H,8.8854907145,-1.4181450762,-1.2240915848\H,7.7098451102,-0.64591
33799,-2.3279934363\H,8.2701604425,0.2252979071,-0.8726334887\C,7.2746
015547,-1.6177010875,1.0088617011\H,7.6517141329,-0.6914520731,1.47981
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399445,1.0374115738\C,3.1755601476,1.2665963507,2.6586643372\H,2.40738
301,0.5158210664,2.4125018765\H,4.0506964915,0.7400665672,3.0807307396
\H,2.7676537944,1.927035709,3.4456796654\C,4.6158910445,3.154506484,1.

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7318174161\H,4.843373081,3.7708828813,0.8434533937\H,4.2580554942,3.82
75889194,2.5325879008\H,5.5603754619,2.6933932079,2.0755786212\C,3.651
7845765,1.2263576326,-4.3563033328\H,3.6636260236,2.2553084275,-3.9577
713293\H,4.6967640136,0.9350901383,-4.5731610548\H,3.0941016033,1.2369
79519,-5.3111684644\C,2.921356181,-1.1715908075,-3.9680635049\H,2.2743
783552,-1.1546207046,-4.863777614\H,3.9120880931,-1.5475425148,-4.2845
65515\H,2.4794130915,-1.8780833287,-3.2479134767\C,-2.9935567482,-2.97
39228812,2.2226451359\H,-3.6399267452,-3.8702843153,2.1923027989\H,-2.
1909311782,-3.0893610858,1.4763679249\H,-2.5317781648,-2.9319525109,3.
2253016541\H,-3.0838563418,-0.8417728122,2.0661828876\\Version=ES64L-G
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E-2a/1c (Type II; conf1)
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15\0\\#p tpsstpss/def2svp/w06 densityfit empiricaldispersion=gd3 opt s
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,-1.0360614112\O,-1.5570661536,0.4191121977,-1.4006662813\O,0.70319595
75,0.4772366402,-0.1657760999\O,0.3137427998,-1.0172412323,-2.34882173
64\O,-0.6957637612,-1.5981534853,0.0438642701\C,-1.4408930409,2.298033
2259,0.0694880858\C,-2.1235327275,1.1703936732,-0.3920369437\C,-3.4206
929358,0.791807267,0.0752486622\C,-4.0016451502,1.5712080763,1.0669351
501\H,-5.0061591326,1.3259980129,1.4265705143\C,-3.3138734393,2.670100
3313,1.6570112351\C,-2.0051107643,3.0345187312,1.1726460019\C,-1.30239
60309,4.0794977225,1.8452109896\H,-0.2915783918,4.339449818,1.51757815
81\C,-1.8721969241,4.7497304487,2.9180735105\H,-1.3082500691,5.5401702
008,3.4254459897\C,-3.1772928725,4.4146137855,3.3693613696\H,-3.618070
5198,4.9552641769,4.2140070781\C,-3.8803316916,3.3931589443,2.74985654
02\H,-4.8786704816,3.1095258545,3.1019632459\C,-0.147431271,2.68627279
31,-0.5619745732\C,0.9028692306,1.7637587322,-0.6236788895\C,2.2232489
206,2.1243263932,-1.0404498356\C,2.4354489163,3.41894835,-1.4937487849
\H,3.4445803092,3.7283139289,-1.7856369978\C,1.3732088192,4.3645894719
,-1.5865511023\C,0.0586920824,4.0007677631,-1.1176348869\C,-0.99555563
46,4.9543103489,-1.2545164875\H,-2.0065495796,4.6808795333,-0.93852976
03\C,-0.7586849291,6.2096287843,-1.7951674443\H,-1.5851955664,6.921557
9418,-1.8975155204\C,0.5444852505,6.5777171026,-2.225055765\H,0.719165
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7\H,2.5931383064,5.9353170113,-2.4669427153\C,3.9225744728,-4.48481318
93,-0.8256743025\C,4.5001347385,-4.3980475686,0.4569075245\H,5.5024314
78,-4.8054240722,0.6268106984\C,3.8282245835,-3.7793473319,1.513569372
8\H,4.3259302561,-3.7275617957,2.4846230681\C,2.5385415214,-3.21917330
89,1.3302633587\C,1.9388433299,-3.350761882,0.0496819669\H,0.932609681
4,-2.9663935025,-0.1373458317\C,2.620012098,-3.9636866639,-0.99846472\
H,2.1355616755,-4.0305099515,-1.9785001475\C,1.8748246039,-2.529241920
9,2.4455058322\C,2.5612487963,-2.4415192745,3.7779068398\H,2.093823872
1,-1.6903491142,4.4282068667\H,3.6184651266,-2.1729173216,3.6312853088
\H,2.5340604071,-3.4200016454,4.2894375125\N,0.6970826641,-1.957253993
8,2.2716835073\H,0.2444711661,-1.8782454266,1.2991313172\C,-0.10174962
27,-1.3104393111,3.2673638007\C,-0.6061572591,-0.0286377764,2.97831107
62\H,-0.3599835491,0.4492918672,2.0265128869\C,-1.4152948705,0.6176210
124,3.9214725547\H,-1.7951533344,1.6202523243,3.7044792307\C,-1.741685
9682,-0.015834654,5.1310543644\C,-1.2573537271,-1.3064261217,5.3989942
159\H,-1.5242456356,-1.8141440868,6.3317919883\C,-0.4378035768,-1.9603
978091,4.4696055734\H,-0.0813671279,-2.976498328,4.6609525941\C,3.3588
144849,1.1587473434,-0.8678568691\C,3.8006250174,0.3429631015,-1.94456

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15348\C,3.9981298477,1.0768466151,0.3949996218\C,4.8916766724,-0.51605
98331,-1.7337727753\C,5.0882376593,0.1977055742,0.5568264914\C,5.55722
62429,-0.6041297275,-0.4951473507\H,5.2390341728,-1.1482719355,-2.5589
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176246,-0.5173297553\C,-4.3626884464,-1.5535106091,0.2650609551\C,-4.5
944039551,-0.3308687641,-1.8592926219\C,-5.0889593091,-2.6164292048,-0
.3013270825\C,-5.3101260011,-1.4257542536,-2.3798995859\C,-5.577643163
2,-2.5747073377,-1.618901317\H,-5.2713931718,-3.510675919,0.3055573771
\H,-5.6765941914,-1.3804719063,-3.4130416494\H,-2.3816181166,0.4926070
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7677,-4.3168937225,-2.763218045\H,5.6416218198,-5.4999562942,-1.678939
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873027,-2.7535724329\H,-3.7792301411,1.6283292118,-2.1810428407\C,-3.8
344181243,-1.6946595897,1.6948436949\C,-6.3621256179,-3.7428902288,-2.
2097973495\H,-6.6400260656,-3.457446054,-3.2420024662\C,-4.9664850863,
-1.5447101987,2.7324111944\H,-4.5612699027,-1.6026452151,3.7594684556\
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83904\H,-8.2508029482,-4.8135332151,-1.902533313\C,-5.4997269133,-5.01
93502883,-2.2925977486\H,-6.0638043654,-5.8412795574,-2.77075362\H,-4.
5821264342,-4.8437741215,-2.8820189561\H,-5.1953407218,-5.3602161617,-
1.2858407249\C,-3.5380319659,0.5262490016,-4.0047724117\H,-4.083255358
4,-0.1787314221,-4.6593793629\H,-3.320720341,1.4338138991,-4.597936952
6\H,-2.578321078,0.0654588611,-3.7164517799\C,-5.6966783771,1.56821001
06,-3.1312304363\H,-5.5109742905,2.4800451927,-3.7282394077\H,-6.33739
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37716\C,6.7637426357,-1.534835694,-0.3630981679\H,6.4754512406,-2.4915
337478,-0.8414844351\C,3.1344828148,0.4250518706,-3.3184999657\H,2.103
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391,-1.1531653708\H,8.8232927043,-1.6688449126,-1.1144720742\H,7.71134
58986,-0.8040779326,-2.2144860079\H,8.2928994043,-0.0042408614,-0.7264
340967\C,7.1700433303,-1.8394631591,1.0867395596\H,7.577870536,-0.9437
930868,1.5902813271\H,6.3162853453,-2.2054667297,1.682367381\H,7.95561
84883,-2.6158926356,1.1055405256\C,3.0688467018,1.0352848629,2.7569758
536\H,2.2851002168,0.3369835249,2.4227993005\H,3.9022178752,0.44353813
44,3.1769782115\H,2.6510015174,1.6552928349,3.5711740628\C,4.623335319
3,2.919940203,2.0284407004\H,4.918168605,3.5816042333,1.194185677\H,4.
2525871705,3.5538348955,2.8548408208\H,5.5301240548,2.3974913196,2.385
2397263\C,3.8677956851,1.4451444639,-4.2166152121\H,3.8950685138,2.447
124562,-3.7548067234\H,4.9120356292,1.1274929181,-4.3968488155\H,3.363
8310662,1.5343018536,-5.196831029\C,3.0239254651,-0.9383167969,-4.0239
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15898625,-4.3254412838\H,2.5251147766,-1.673098674,-3.3726102655\C,-3.
0734963099,-3.0196596902,1.9018253689\H,-3.7411567227,-3.8963185221,1.
81181147\H,-2.2615966376,-3.1137193344,1.1627345183\H,-2.6282928693,-3
.0455439729,2.9123679317\H,-3.1123776141,-0.8788302257,1.8642763009\\V
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=2.118e-06\Dipole=2.7055997,-1.8058762,4.6562416\Quadrupole=-0.6702615
,2.8556223,-2.1853608,-22.5056812,1.7057,-8.9444242\PG=C01 [X(C65H72N1
O4P1)]\\@

E-2a/1c (Type II; conf2)
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015\0\\#p tpsstpss/def2svp/w06 densityfit empiricaldispersion=gd3 opt

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809,0.5217828828,-0.1187704196\O,0.3240243179,-1.1080942874,-2.2098112
907\O,-0.6514035879,-1.5891903612,0.219774817\C,-1.5493342787,2.248431
4576,0.0748253162\C,-2.1843067218,1.0728178766,-0.3317482048\C,-3.4504
548049,0.6451026954,0.1778757969\C,-4.0503655797,1.4332314209,1.150947
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46\C,-2.0421670899,4.7705680099,2.8518504313\H,-1.507854213,5.60316086
93,3.3225499006\C,-3.3188940357,4.3860849892,3.3431474928\H,-3.7677291
003,4.930220563,4.1812789694\C,-3.9835192865,3.3126532657,2.7710043046
\H,-4.9582519201,2.990996503,3.1549427723\C,-0.286403047,2.6699704735,
-0.5967463913\C,0.8015407412,1.791563414,-0.6423074704\C,2.0932560465,
2.1843348638,-1.1152896749\C,2.2380254328,3.4627632728,-1.6354023316\H
,3.2246483557,3.7979513338,-1.9722916774\C,1.1356998657,4.3606861088,-
1.73637161\C,-0.1499963626,3.9652240232,-1.2152012588\C,-1.2442139849,
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C,-1.07438808,6.1093952726,-1.9613670212\H,-1.931533868,6.7835022772,-
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569488165,-3.1830179538\H,-2.1539894261,0.6065293282,6.0422878621\C,4.
532773395,-5.1757686648,-1.9631433834\H,4.6161011095,-4.4801810731,-2.
8191853148\H,5.5414915928,-5.5441256216,-1.7161970914\H,3.9182299703,-
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7,1.9484861916\C,-6.0892105591,-4.1954568341,-1.8339392254\H,-6.159182
6018,-4.9012845215,-0.9849125419\C,-4.8911117297,-1.6261566694,2.97098
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.8288618155\H,-4.2476070482,-5.1257552613,-2.5901038142\H,-5.751825622
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4911354,-1.5083070064\H,-7.5215969046,-3.1989591277,-3.1721855485\C,-3
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4.5047732624\H,-3.4383175501,1.0513373899,-4.5304946956\H,-2.594981271
7,-0.2246981591,-3.6035419752\C,-5.7968153858,1.0964700094,-3.03282678
74\H,-5.6817154008,1.990751445,-3.6726652048\H,-6.3956865988,0.3550067
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22817,-1.1683979567,-0.2998710966\H,6.6740095865,-1.7343835426,0.63783
30168\C,3.049373087,0.4448418658,-3.346011166\H,2.0048992437,0.7581924
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47\H,8.0101637097,-2.8187440259,-1.1137243237\H,6.2960608802,-2.847968
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78232,-0.2429184261,-0.0639362831\H,8.2709988943,0.3574372811,-0.96793
86415\H,7.8816671949,0.4553181508,0.7729885389\H,8.9606372117,-0.83634
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9\H,2.6644924563,1.9094973427,3.5353797904\C,4.459039823,3.2317502366,
1.8341170236\H,4.65733463,3.8687311045,0.9533681713\H,4.0791555022,3.8
793489473,2.6457642239\H,5.4226300305,2.8021936758,2.1657505459\C,3.70
21783605,1.4542230074,-4.3145333394\H,3.6895247366,2.4777235484,-3.901
9883859\H,4.7556735226,1.1821188876,-4.5141064169\H,3.1643044308,1.470
3197289,-5.2806234955\C,2.9940397738,-0.9593940278,-3.9754999771\H,2.3
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3.0080320172,2.2374283889\H,-3.4939664999,-3.9344407026,2.1912324703\H
,-2.0640915054,-3.0852873803,1.5148059857\H,-2.4616828479,-2.944500891
8,3.2525596487\H,-3.0800867724,-0.8830379563,2.0746201863\\Version=ES6
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Dipole=2.8358753,-1.5972804,4.5791249\Quadrupole=-0.2399068,0.8264343,
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@

Z-configuration

Z-2a/1c (Type II; conf0)
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,-1.690068728\O,-2.1419846958,0.9699931365,-1.1245056325\O,0.391113577
3,0.7583457809,-0.6191392296\O,-0.5934618898,0.6102244498,-3.106179937
\O,-0.8663764429,-1.3130943639,-1.2876427036\C,-1.6016610808,1.8888461
214,1.0066390326\C,-2.3731778268,1.0197229608,0.2347930461\C,-3.433470
7899,0.224563718,0.7709174107\C,-3.6729075092,0.3092190306,2.136386880
5\H,-4.4952591045,-0.2646950688,2.5755884857\C,-2.8575126094,1.1001909
848,2.9960213631\C,-1.7892386463,1.8911695511,2.4353832865\C,-0.929917
5547,2.5988716089,3.3292790364\H,-0.0890704771,3.168883285,2.923308388
4\C,-1.1316917201,2.5524140962,4.7012435502\H,-0.451331549,3.093220364
3,5.3682298836\C,-2.2076387844,1.8034246781,5.2493989433\H,-2.35933537
52,1.7801611651,6.3340152602\C,-3.0508390303,1.0914717453,4.4105187909
\H,-3.8705226485,0.491271111,4.8216026503\C,-0.5600932025,2.7323068562
,0.3539329384\C,0.463340096,2.1154951411,-0.372369691\C,1.6474740538,2
.8148174573,-0.7699276191\C,1.6747441333,4.193661125,-0.6057547347\H,2

S38

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385963993\C,-0.5492981412,4.166653676,0.4781535357\C,-1.6279097168,4.8
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21653012\C,-0.4761648775,7.0040626755,0.6528415142\H,-0.4599094538,8.0
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48696,2.6407269114\C,3.8515279517,-2.7292228695,1.2315257455\H,3.34168
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647,-1.4057964098\C,5.2011600169,-4.8761847916,0.0450681258\H,5.718161
3481,-5.723033997,-0.4193784304\C,2.0739278515,-2.821237389,-0.5455859
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12916,-2.3702538538\H,2.216678429,-3.6615908983,-2.5097498646\H,2.8223
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7533,-1.1430914298\C,3.1433828247,1.6490375191,-2.4795331647\C,3.78389
4742,1.6920543437,-0.0985668848\C,4.3075356785,0.9026358321,-2.7476164
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,-3.1419874795,-3.8069579219,2.819681345\H,-4.4243459075,-2.5661263175
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23,-3.9505459699,-1.6811445071\H,-7.3131019632,-4.6572739602,-1.029371
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,2.0975222292,-3.6125574001\H,1.2109319966,2.2053097988,-3.1848325504\
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Z-2a/1c (Type II; conf1)
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S40

069652858,-0.6862419093,1.5223967976\C,-0.148710959,-1.7395842378,3.42
48096885\H,-0.6779196451,-0.9329995909,3.9415112957\C,0.195038896,-2.9
165476223,4.1067936287\C,0.8575601297,-3.9535201593,3.4265399152\H,1.1
05301792,-4.8834363343,3.9491091358\C,1.1982636266,-3.8127122281,2.076
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6063854,-1.0685469179\C,3.0307868696,1.912443542,-2.4352503593\C,3.733
6649535,1.8170526994,-0.0738254213\C,4.2148268603,1.232962589,-2.78298
99821\C,4.8938174652,1.1287466851,-0.4716703291\C,5.1536321723,0.82501
18072,-1.820522845\H,4.4186414958,1.013056753,-3.8369939915\H,5.618398
945,0.8236900943,0.2912327306\C,-4.2208040099,-0.8365853502,-0.0547897
018\C,-4.0830815998,-2.2513328215,-0.0664356816\C,-5.1689617709,-0.208
4942537,-0.9093664698\C,-4.9276134741,-3.0072054284,-0.902962007\C,-5.
9800701745,-1.0083311958,-1.7332103174\C,-5.8849606813,-2.4113019178,-
1.7391418134\H,-4.8317795398,-4.0996938451,-0.9099611972\H,-6.71352586
73,-0.5193523229,-2.3853362656\H,-0.0640267275,-3.0327744572,5.1644171
408\C,7.301940447,-4.5867541371,1.4280149219\H,7.238850196,-4.84559982
92,2.5003569884\H,7.6928989244,-5.4578094892,0.8772745738\H,8.03766430
77,-3.7649894166,1.3395593348\C,-5.3518318996,1.3104022803,-0.94482818
99\H,-4.6280251227,1.7575162368,-0.242900121\C,-3.0379277891,-2.971628
7294,0.7881084407\C,-6.7804976568,-3.2620736038,-2.6359884382\H,-6.530
9458722,-4.3206243982,-2.431768818\C,-3.6795101802,-3.6514735276,2.015
5690728\H,-2.9061583924,-4.1398498539,2.6366401404\H,-4.2169291071,-2.
9249601367,2.6493374329\H,-4.4040145732,-4.4266538725,1.702797737\C,-6
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954,-3.6547864765,-4.7664177396\C,-8.274676988,-3.0626645717,-2.308896
8281\H,-8.9008656105,-3.7310778108,-2.9280463707\H,-8.4845436422,-3.28
27438765,-1.2468203759\H,-8.5937159956,-2.0234568841,-2.5100958164\C,-
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,1.6041841863,-2.6670597176\C,-6.7582270649,1.7172636506,-0.4588160315
\H,-6.8577098921,2.8181311,-0.4384620034\H,-7.5463681871,1.3201453469,
-1.1246349949\H,-6.9514180824,1.3372263918,0.5605952051\C,6.4284165339
,0.0945583532,-2.2356414103\H,6.378338113,-0.0435316633,-3.3322478437\
C,2.0589693727,2.3930396908,-3.5113241089\H,1.0573868076,2.4281929507,
-3.0495080355\C,3.4897929348,2.1144655089,1.4097570065\H,2.7760305402,
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4146809231\H,7.7951131498,1.0993923619,-0.8382622145\C,6.5245822093,-1
.3026062887,-1.5905676741\H,6.6008198443,-1.2313274109,-0.4907372136\H
,5.6375040054,-1.9148583626,-1.8277586813\H,7.4189246554,-1.8409282839
,-1.9542920353\C,2.8213144265,0.911962699,2.1072754387\H,1.9423108828,
0.5649890515,1.5416048339\H,3.5298113001,0.0687001834,2.1896072741\H,2
.4914518922,1.1794449651,3.1276135117\C,4.7595250034,2.5522045792,2.16
26050977\H,5.2523253626,3.4061631207,1.6637932603\H,4.5003926841,2.860
3091573,3.1917788494\H,5.4966309998,1.7324251815,2.2427109205\C,2.4307
371747,3.8204737934,-3.9687519428\H,2.4373211862,4.5270014572,-3.12038
77784\H,3.4355628698,3.8364158139,-4.4309967909\H,1.704100315,4.190816
0484,-4.7154447961\C,1.9538788644,1.443185534,-4.7161279264\H,1.143245
0904,1.778533444,-5.3870565527\H,2.8855281809,1.4185536228,-5.31148851
8\H,1.7127646776,0.4173113149,-4.3916024145\C,-2.216507599,-3.98953373
04,-0.0280564672\H,-2.8320051653,-4.8479040423,-0.35457374\H,-1.778874
5533,-3.5082406204,-0.9172430602\H,-1.3933477996,-4.390340802,0.590438
1083\H,-2.332630643,-2.2072078206,1.1544705283\\Version=ES64L-G09RevD.
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25.1282264,-3.7225466,5.1459388\PG=C01 [X(C65H72N1O4P1)]\\@

Z-2a/1c (Type II; conf2)
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scrf=(smd,solvent=ch2cl2,read)\\title\\0,1\P,-0.7676123827,0.194499547
9,-1.650117495\O,-2.044234111,1.0901298303,-1.0386692588\O,0.445910937
6,0.6415723985,-0.5512853515\O,-0.5383755627,0.6970892848,-3.043050722
\O,-0.9521656052,-1.2879061433,-1.321791423\C,-1.4772690065,1.79581836
78,1.169851827\C,-2.3011731543,1.0591299109,0.3159837585\C,-3.44243268
21,0.3232259072,0.7643566472\C,-3.726683887,0.3399909342,2.123007208\H
,-4.6119752619,-0.1856557649,2.4949594166\C,-2.8785744202,0.9970539193
,3.0597346477\C,-1.7180477967,1.7135845923,2.5909467461\C,-0.830543572
9,2.2656476584,3.5637089413\H,0.0784959299,2.7724854559,3.229526362\C,
-1.0939119809,2.1525276182,4.9212419826\H,-0.3907817521,2.5761832485,5
.6466940891\C,-2.2624518744,1.4864993478,5.3783928142\H,-2.4633092526,
1.4104749993,6.4525672371\C,-3.1331866455,0.9173674473,4.4623933863\H,
-4.0243250619,0.376439326,4.8003695957\C,-0.3432750546,2.5878667268,0.
6134919861\C,0.6242118992,1.9567610299,-0.1776535267\C,1.8775189294,2.
5724573302,-0.4949048115\C,2.0673634123,3.8958268829,-0.1244732469\H,3
.0212382409,4.3855423882,-0.3453196726\C,1.0524205219,4.6434656617,0.5
40300652\C,-0.1732740943,3.9863577234,0.9199078997\C,-1.1819863718,4.7
608843665,1.5692972247\H,-2.1305612556,4.2848994705,1.8345517986\C,-0.
9816693173,6.1042804782,1.8506937707\H,-1.7743103581,6.6800368624,2.34
11361999\C,0.2392954411,6.7421138483,1.502344274\H,0.3870200997,7.8020
459409,1.7364158035\C,1.2329036926,6.0236635322,0.8559297813\H,2.17434
97544,6.5063360877,0.569619268\C,5.6167263017,-3.9556972874,1.57733744
16\C,4.7816249733,-2.9529517955,2.1216559415\H,5.0725874153,-2.4524207
445,3.0518982364\C,3.5928014425,-2.5837870923,1.494104459\H,2.97290637
23,-1.7993624775,1.9337526228\C,3.2072796604,-3.1867204284,0.271697257
1\C,4.0480494376,-4.1720979221,-0.2900513836\H,3.7766172288,-4.6587545
137,-1.2313835446\C,5.2211344917,-4.560258839,0.3675291997\H,5.8481243
159,-5.3418626279,-0.075023265\C,1.9985694502,-2.7277331431,-0.4397242
265\C,2.0562398401,-2.4981496016,-1.9184299884\H,1.0698271065,-2.22799
65215,-2.3211965693\H,2.4326763485,-3.4009861262,-2.4287474895\H,2.777
3057297,-1.6859319066,-2.1241668965\N,0.8771700799,-2.4278841492,0.171
5089134\H,0.1093479449,-1.951665285,-0.4344321936\C,0.5095011631,-2.63
04213852,1.5379068449\C,-0.1533167676,-1.5795744305,2.1953173957\H,-0.
3398021799,-0.6412377114,1.6664181921\C,-0.5571254105,-1.7485336168,3.
5263857748\H,-1.0608460604,-0.9259370739,4.042926376\C,-0.3241777443,-
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.4763050558,-4.9777559685,4.0146053494\C,0.7316180173,-3.8609393863,2.
183460238\H,1.2161522585,-4.6823509595,1.6483597968\C,2.9789659973,1.7
611719847,-1.1138453113\C,3.0870357575,1.675661021,-2.5290375327\C,3.9
144096411,1.0785975568,-0.2856018096\C,4.1242773854,0.907062991,-3.090
5617815\C,4.9270479169,0.3166840652,-0.9031808247\C,5.0559464539,0.217
1910928,-2.2981825642\H,4.2151594578,0.8423149769,-4.1804407204\H,5.63
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\C,-5.9474897537,-0.4215955731,-2.0083815417\C,-5.9971367572,-1.824536
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897524,-3.4937798717,2.2916934062\C,-5.1288239612,1.8257102525,-1.1798

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659404438,0.7178401886\C,-6.8939450244,-2.5745764178,-2.9929712775\H,-
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,1.8983178942\H,-3.5444325123,-3.8010810326,2.5871232578\H,-4.73501766
5,-2.4726377787,2.4763329077\H,-4.9835339675,-3.9706984079,1.538284833
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8589\H,-6.7092215636,-3.8718213507,-4.7515320181\H,-5.3372885381,-2.74
25093195,-4.5337011155\H,-5.4835802022,-4.1848068742,-3.4894544527\C,-
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3553960431\H,-4.6115938111,3.4553394591,-2.5448280477\H,-3.6695940722,
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,-1.5134266979\H,-6.8177465417,2.0412096136,0.209477438\C,6.1762666377
,-0.5993006494,-2.9370847395\H,6.0354605196,-0.53750818,-4.0325607782\
C,2.134699222,2.4577212668,-3.4354512437\H,1.1718055405,2.5400452312,-
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2762720902,1.5347513337\C,7.5608985737,-0.0030809691,-2.6087568446\H,8
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.9271350037\H,7.7635242891,-0.0430151875,-1.5225055011\C,6.1049729784,
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9231739552,2.3747659356,2.8022701927\C,2.6571793371,1.0216622811,2.026
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644\H,3.6448869409,3.8481508447,-4.2136014255\H,1.9669062391,4.4640061
071,-4.3036658417\C,1.8419915056,1.7543744159,-4.7719014422\H,1.044019
6858,2.295933157,-5.3106030002\H,2.7280612574,1.7328702797,-5.43329243
79\H,1.4895579214,0.7238186372,-4.6056488419\C,-2.6580660017,-3.775883
5291,-0.0332524335\H,-3.3382138691,-4.566019828,-0.4011896366\H,-2.108
9488098,-3.3536681105,-0.8899420512\H,-1.9299022844,-4.2573218852,0.64
43803216\H,-2.6632045378,-1.9803883691,1.1328636749\\Version=ES64L-G09
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e=4.2240919,-3.6393994,3.7143654\Quadrupole=8.190859,7.1964211,-15.387
2801,-22.1103806,-1.4429095,2.4644772\PG=C01 [X(C65H72N1O4P1)]\\@

Z-2a/1c (Type II; conf3)
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crf=(smd,solvent=ch2cl2,read)\\title\\0,1\P,-0.8166798526,0.0155588802
,-1.630833863\O,-2.1807228347,0.8671760311,-1.1594872795\O,0.331144657
8,0.6993999063,-0.5788491975\O,-0.5900200712,0.3630482362,-3.071584643
7\O,-0.898132429,-1.424867239,-1.1248670147\C,-1.6830368518,2.02357477
83,0.8658789284\C,-2.4378172334,1.0698863945,0.1800705676\C,-3.5115855
912,0.3381448519,0.7775872305\C,-3.7826559141,0.575776686,2.1190414955
\H,-4.6107092955,0.0470845912,2.6023468327\C,-2.9883964061,1.462832263
6,2.901638089\C,-1.9089988078,2.1911141697,2.279988443\C,-1.0802501739
,3.007583587,3.1079297133\H,-0.2339283482,3.5363282627,2.6606811685\C,
-1.3192243935,3.1214394344,4.4697980092\H,-0.6618237777,3.7454384109,5
.0851439242\C,-2.4034707071,2.4302485442,5.0740742155\H,-2.5851785414,
2.5327158814,6.1494955902\C,-3.2177803788,1.6160240426,4.3025925721\H,
-4.0454651155,1.0619090968,4.7598775915\C,-0.6142268707,2.779644915,0.

1514547869\C,0.4199854866,2.0734896396,-0.4710546947\C,1.6344777523,2.
7045197611,-0.8929609439\C,1.6932192866,4.090936782,-0.8613527333\H,2.
6170288522,4.5975889979,-1.1605927705\C,0.5920869958,4.8775011653,-0.4
117775489\C,-0.572651377,4.2191386773,0.1282688204\C,-1.6546424257,5.0
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71757891\C,-0.4319063728,7.0584709431,0.0207308946\H,-0.3897769441,8.1
526112371,-0.0143212304\C,0.6336911749,6.3033724079,-0.4442170868\H,1.
5271533964,6.7906680845,-0.850906914\C,6.0370818461,-3.5861072863,1.31
82358443\C,5.2054753995,-2.5759943466,1.8525240544\H,5.5635274622,-1.9
674574067,2.6903909121\C,3.9398409017,-2.3278848702,1.3236098398\H,3.3
288613612,-1.5248810641,1.7404917308\C,3.4620822073,-3.0724833121,0.21
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.1783107309,-5.1183506551,-0.2123234037\C,2.1680981983,-2.741498249,-0
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-2.5008423223,-2.2227843144\H,2.3764174852,-3.6984514279,-2.3104178325
\H,2.7527108409,-1.9615008821,-2.2968925873\N,1.1017360294,-2.38081108
39,0.2726105101\H,0.2762502913,-1.9926744222,-0.3152016375\C,0.8304490
726,-2.4043655535,1.6736276879\C,0.0474022111,-1.3550464018,2.18859463
61\H,-0.2768751497,-0.5499145929,1.5242663446\C,-0.3026373928,-1.35659
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1608\H,1.1729630496,-4.299735697,4.4899148384\C,1.2311816985,-3.473916
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-2.5706581706\C,4.7437876444,0.6402486127,-0.2329746542\C,5.0130389289
,0.0520180346,-1.4831395817\H,4.408833211,-0.0019629002,-3.5587427511\
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8.1217466759,-3.0650035786,1.4758489614\C,-5.2675793809,1.2932463007,-
1.4430431394\H,-4.5775687519,1.861414743,-0.7970179006\C,-3.3167743815
,-2.5932266957,1.3585322064\C,-6.6779408305,-3.4976666497,-2.340375542
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3323482347,-4.9099438891,-2.0752052658\C,-5.7783960748,-4.4891266934,-
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47,-3.957305142,-3.7666378339\H,-5.1898073584,-5.1143056497,-2.4106699
934\C,-4.8606007786,1.5733912393,-2.9037569421\H,-5.5462756132,1.08081
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57498467,1.2154548242,-3.0985393642\C,-6.6909670821,1.8105811644,-1.14
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.6961234059\C,2.283538457,1.7237362417,-3.6371520204\H,1.2633358371,1.
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,1.605091327,0.95803297,1.6542110665\H,3.0369576281,0.3330517606,2.513
2260937\H,2.1980762199,1.7830070766,3.1237085145\C,4.7224817023,2.4900
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35,3.0428170654,3.0314783058\H,5.278937681,1.5826048124,2.4030181373\C
,2.8532796031,3.0240197623,-4.2465380484\H,2.8843672667,3.8379423071,-
3.5014128854\H,3.8830236509,2.8651688016,-4.6182506349\H,2.2311709446,
3.3622339583,-5.0958759732\C,2.1511492592,0.6308330927,-4.7101325004\H
,1.4320695718,0.9542242039,-5.4835277227\H,3.1118219907,0.4264791251,-
5.2182877376\H,1.7704403067,-0.307357594,-4.2740621913\C,-2.4099234109
,-3.7258635246,0.8371396576\H,-2.9926171939,-4.6202190081,0.549224578\
H,-1.8345692187,-3.3834764674,-0.0380188824\H,-1.6989008108,-4.0327793
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06\Dipole=4.5321613,-3.1826639,3.6425749\Quadrupole=11.0306626,7.19329
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Z-2a/1c (Type I; conf0)
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5,0.6684969477,-0.5685879305\O,-0.7933787212,0.1177798753,-2.948977614
4\O,-0.9962795819,-1.4670307343,-0.8157171617\C,-1.6426839449,2.023946
5707,0.9725275202\C,-2.4488982872,1.0720365854,0.3474539537\C,-3.51403
85802,0.3827796516,1.0075837656\C,-3.7140399715,0.6550473949,2.3555933
083\H,-4.534148431,0.1626331029,2.8888022324\C,-2.8616236107,1.5392739
8,3.0792593286\C,-1.7957801759,2.2271335539,2.390797635\C,-0.913490889
,3.0481856018,3.1564453856\H,-0.0760622133,3.5426189036,2.6555045462\C
,-1.0931237714,3.2106696127,4.5225095664\H,-0.3979354288,3.838828961,5
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.7066485187,6.2699182085\C,-3.0284168314,1.7425967377,4.4827354374\H,-
3.8480568186,1.2230400758,4.992182311\C,-0.6190969887,2.7605269146,0.1
767580716\C,0.369139991,2.0451200088,-0.5085480208\C,1.5356108945,2.67
58160295,-1.0473612215\C,1.5875120155,4.0631586953,-1.0473067094\H,2.4
790518892,4.567735051,-1.4350049498\C,0.5252348197,4.8534451985,-0.519
5525091\C,-0.5894173889,4.1998508852,0.1216470427\C,-1.6360813677,5.01
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780289693,6.3958998135,0.5735972028\H,-2.3974664581,6.998192704,0.9811
893201\C,-0.4689792772,7.0383162715,-0.0396668835\H,-0.4334003639,8.13
19247866,-0.0933680957\C,0.5587098534,6.2790334676,-0.576987775\H,1.41
52570265,6.7622814401,-1.0606649176\C,5.0083124262,-3.1014191224,3.741
7252019\C,5.0387516221,-2.638632073,2.4059081635\H,6.0032234575,-2.480
531465,1.9109487048\C,3.8636469102,-2.3750353175,1.7045991732\H,3.9240
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30464\C,2.5658400647,-2.9709914476,3.6747843652\H,1.6070398395,-3.0982
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6787\C,0.2239801446,-1.5623753191,2.3961286719\H,-0.5506862359,-1.1944
395868,1.708506082\H,0.5983888034,-0.7399046714,3.0265633648\H,-0.2250

S45

969492,-2.3157548017,3.0688543447\N,1.1695932576,-2.354279442,0.345867
7364\H,0.258432894,-1.9465806675,-0.0864297288\C,1.9843654975,-3.03211
43591,-0.6138271751\C,2.2485375698,-2.3718428749,-1.8258973185\H,1.899
8883777,-1.346646104,-1.9775400629\C,2.9919449968,-3.0290004055,-2.815
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.5386240103,-6.0089560773,-1.2162820555\C,2.4381854174,-4.3440669931,-
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1.8391943931,-1.4062490807\C,2.9146979743,1.3229421171,-2.7136740983\C
,3.6807213646,1.5644271618,-0.3818495286\C,4.0461690826,0.5252116467,-
2.9706285312\C,4.7839375238,0.7460560338,-0.6864139014\C,4.9842774839,
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,5.5127073819,0.5242266807,0.1001279279\C,-4.3741892637,-0.5807365274,
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4,-0.1092926593,-0.8015718668\C,-5.207734252,-2.8400216709,-0.13729569
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405979,-1.174143667\H,-5.2006240199,-3.9050515559,0.1224597974\H,-6.67
53707542,-0.6627513625,-2.2941414323\H,4.0446673639,-4.8428775748,-3.3
721537672\C,6.2894332002,-3.4096544308,4.4751220265\H,6.9952025905,-2.
5617294413,4.4118107097\H,6.1051239684,-3.6357052247,5.5379939253\H,6.
7964224058,-4.2816379957,4.0203936997\C,-5.2891392721,1.3692730743,-1.
1882153574\H,-4.5569999829,1.9225183452,-0.5772529914\C,-3.4611054457,
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-7.4689479233,-2.7750207033,-2.7142228726\C,-4.2792087707,-3.016948557
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,-4.0471932633,-3.3147276135\H,-5.6221636785,-5.1125405607,-1.89952924
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03381412\C,1.9320869324,1.6727503711,-3.8309165215\H,0.9481719776,1.83
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6,1.7165653477\H,5.4470174977,3.1624575895,1.0796277216\H,4.6316471434
,3.0300899401,2.6653318259\H,5.4363726555,1.6079821911,1.963823288\C,2
.3534647569,2.9885068292,-4.5209413189\H,2.4224932192,3.8186364399,-3.
7964861971\H,3.3412397167,2.8784706002,-5.0064266277\H,1.6194860391,3.
27345864,-5.2973164887\C,1.7451968328,0.549171382,-4.8642284979\H,0.94
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6911754623,1.1210874359\H,-3.1751406678,-4.5663456302,0.8142385076\H,-
1.9893165158,-3.3428352312,0.2538801435\H,-1.8710158068,-4.0333857723,

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Z-2a/1c (Type I; conf1)
1\1\GINC-WORKER\FOpt\RTPSSTPSS\def2SVP/W06\C65H72N1O4P1\JHIOE\31-Oct-2
015\0\\#p tpsstpss/def2svp/w06 densityfit empiricaldispersion=gd3 opt
scrf=(smd,solvent=ch2cl2,read)\\title\\0,1\P,-0.9603916882,-0.14192555
16,-1.4145448894\O,-2.2937923313,0.734318966,-0.9079307935\O,0.2659287
821,0.6562832469,-0.5481198525\O,-0.8688371361,0.061107523,-2.89709500
66\O,-0.9585567758,-1.5205372345,-0.7546655317\C,-1.6727979144,1.95512
93959,1.0400726571\C,-2.4637126007,0.9751343884,0.4394334874\C,-3.4865
993364,0.2526748334,1.1303319784\C,-3.6601383198,0.5238729348,2.482266
008\H,-4.4486756315,0.0058568749,3.0385120653\C,-2.8187311265,1.438835
0964,3.1804065709\C,-1.7951316026,2.1585880225,2.4614381137\C,-0.92116
50732,3.0122251903,3.2005502972\H,-0.115215161,3.5330793747,2.67560386
8\C,-1.0692164709,3.1738760149,4.5704644424\H,-0.3807560553,3.82754964
16,5.1173407247\C,-2.101616696,2.4940502208,5.2709493864\H,-2.21259945
18,2.6356927512,6.3515778234\C,-2.9541629088,1.6413078867,4.5873880748
\H,-3.7420505508,1.0966516627,5.1201498987\C,-0.6932513919,2.720689274
9,0.216506625\C,0.2996050952,2.0346514201,-0.4921824331\C,1.4323008436
,2.7001112095,-1.0605338504\C,1.4417863631,4.0884255032,-1.0623944608\
H,2.3071228295,4.6194357469,-1.4735627378\C,0.3692981597,4.8467627642,
-0.5090437558\C,-0.7094890527,4.1601249935,0.1583114653\C,-1.769045768
9,4.940550149,0.7126914895\H,-2.6091470058,4.4320723454,1.1955000425\C
,-1.7550234675,6.3252140637,0.6310039981\H,-2.5836158766,6.9023007716,
1.0560863859\C,-0.6795417042,7.0007332608,-0.0059526155\H,-0.678206434
5,8.0949241044,-0.059708146\C,0.3582991723,6.2727508812,-0.5667219016\
H,1.1883945855,6.7817879224,-1.0697325253\C,5.2004208155,-3.0250042411
,3.6425576078\C,5.1863514831,-2.5598366175,2.3072965971\H,6.1336525806
,-2.3908437003,1.7833045709\C,3.9880406618,-2.3089943062,1.6412879305\
H,4.0145105629,-1.9286442732,0.6172667652\C,2.7468500902,-2.4940897831
,2.3011227884\C,2.7555882593,-2.9207610335,3.6479806191\H,1.8135834021
,-3.0595213126,4.1868153701\C,3.9637527542,-3.1974412812,4.2967665638\
H,3.9474060319,-3.547970644,5.3345320763\C,1.4725373809,-2.1625659817,
1.641802139\C,0.3529149342,-1.5598303924,2.4366275417\H,-0.4480050231,
-1.2068105017,1.7716706607\H,0.7274446937,-0.7306697357,3.0579924101\H
,-0.0619823536,-2.3231869187,3.1197105752\N,1.2564572151,-2.3337889769
,0.3604043301\H,0.3230545599,-1.9513119898,-0.0481910402\C,2.057246718
6,-2.998027661,-0.6205485917\C,2.2831414743,-2.3322848702,-1.837319491
1\H,1.9180726799,-1.3112166929,-1.9780909738\C,3.0095326036,-2.9787775
3,-2.8462444606\H,3.1956153973,-2.4582359001,-3.791120851\C,3.50133789
28,-4.2775639774,-2.6424694289\C,3.2602594862,-4.9368074736,-1.4248858
288\H,3.6314944569,-5.9549445561,-1.2674517672\C,2.5322465319,-4.30470
19364,-0.4094585057\H,2.3246889706,-4.814993753,0.5356525607\C,2.64149
02848,1.9003943847,-1.4507276546\C,2.8059291398,1.3856395081,-2.761349
2441\C,3.6317016372,1.6617769647,-0.4541659777\C,3.955846426,0.6254978
124,-3.0494237243\C,4.7524026258,0.880210988,-0.7887780858\C,4.9331282
947,0.3498704538,-2.0790197503\H,4.097891056,0.22868043,-4.0606557593\
H,5.5118855366,0.6866550361,-0.0239581668\C,-4.3284943486,-0.747115530
9,0.3980396781\C,-4.2575997979,-2.1285398091,0.7303086403\C,-5.2090676
269,-0.3140736557,-0.6345383435\C,-5.0807757476,-3.037478364,0.0378728
661\C,-6.0021536064,-1.2644359317,-1.3000004923\C,-5.9583648883,-2.632
8340971,-0.97966004\H,-5.0296596373,-4.1027325631,0.2943345483\H,-6.67
97030525,-0.9217058524,-2.0906730476\H,4.0692966679,-4.7792182576,-3.4

329440334\C,6.5053350523,-3.3244606277,4.3364451026\H,7.2071291631,-2.475984841,4.2442552655\H,6.3559675207,-3.543604065,5.4062959985\H,6.9988255468,-4.1990257821,3.8717129947\C,-5.3556007075,1.1591448746,-1.0236118557\H,-4.6335114901,1.7451860148,-0.4311265934\C,-3.3077630412,-2.6708989056,1.7999186443\C,-6.8125174843,-3.6517421718,-1.7287756145\H,-6.6665065028,-4.6268346316,-1.2269134725\C,-4.0802726887,-3.1505692367,3.0464371084\H,-3.3794378572,-3.4931917128,3.8304378942\H,-4.7015053221,-2.3427476817,3.4723403951\H,-4.7496964864,-3.9955509222,2.7994474389\C,-6.339187423,-3.801752377,-3.1901274026\H,-6.4589771131,-2.8527107454,-3.7451302489\H,-5.2731417128,-4.0876116905,-3.2353386377\H,-6.9261968954,-4.5780342609,-3.7148757027\C,-8.3147397644,-3.3111741529,-1.662234861\H,-8.915036775,-4.1046952243,-2.1437290016\H,-8.6549766267,-3.2108258066,-0.6159216899\H,-8.5359189849,-2.3621281805,-2.1842159273\C,-5.0251441065,1.3954773605,-2.511412124\H,-5.7535226746,0.8918995571,-3.1736797595\H,-5.0553426937,2.4761638257,-2.7430810497\H,-4.0162609525,1.0208365883,-2.7515233494\C,-6.7613638159,1.6887172283,-0.6689133542\H,-6.8418503308,2.7648805705,-0.9094205753\H,-7.5471193745,1.1565529627,-1.2362610032\H,-6.9755853934,1.5617079772,0.4076364139\C,6.1754462192,-0.4621806442,-2.4362821044\H,6.004689611,-0.8859385851,-3.4440056214\C,1.7800497671,1.6948259717,-3.8513520135\H,0.8063214497,1.8299086437,-3.3496989631\C,3.4755265452,2.2156816369,0.9667526824\H,2.8478887569,3.1206285995,0.8954918203\C,7.419074427,0.4492905159,-2.5148061378\H,8.3091151099,-0.1256235644,-2.8305159099\H,7.2660874307,1.271213018,-3.2368174661\H,7.6375837332,0.900281993,-1.5290383536\C,6.4146374311,-1.6379994633,-1.468738855\H,6.6388660793,-1.280115614,-0.4473965259\H,5.5331229232,-2.300026018,-1.4169541592\H,7.2764320906,-2.2433274544,-1.8042327075\C,2.7281889645,1.2149975578,1.8741303185\H,1.7742653488,0.8978979391,1.4242299969\H,3.3401352726,0.3114231682,2.0396473974\H,2.511446768,1.6674408036,2.8591646467\C,4.807809555,2.6389239845,1.6124501553\H,5.3754140261,3.3284361323,0.9619797871\H,4.6133094862,3.1549111819,2.5700656843\H,5.4532238255,1.7699416165,1.8361591657\C,2.1403400988,3.0145371586,-4.5676150634\H,2.201703618,3.8556058183,-3.8550873124\H,3.1176578246,2.9305291015,-5.0787968711\H,1.3768862463,3.2661886591,-5.3268845286\C,1.5969844047,0.5534317528,-4.8657629506\H,0.7675080462,0.7949499895,-5.5539643233\H,2.5012550208,0.3943724846,-5.4816550561\H,1.3393131993,-0.3894617245,-4.3563578244\C,-2.3942586498,-3.7860800253,1.2504848269\H,-2.970655633,-4.6889949242,0.9774923456\H,-1.8502203319,-3.4320909112,0.3599384367\H,-1.6558893452,-4.0868985014,2.0166012884\H,-2.6536039064,-1.8415603659,2.1138336781\\Version=ES64L-G09RevD.01\State=1-A\HF=-3216.1217998\RMSD=5.808e-09\RMSF=3.771e-06\Dipole=4.4394202,-2.6783232,4.5048046\Quadrupole=5.8602126,2.1479973,-8.0082099,-18.8575981,3.62146,-8.0502377\PG=C01 [X(C65H72N1O4P1)]\\@

Z-2a/1c (Type I; conf2)
1\1\GINC-LOGIN\FOpt\RTPSSTPSS\def2SVP/W06\C65H72N1O4P1\JHIOE\01-Nov-2015\0\\#p tpsstpss/def2svp/w06 densityfit empiricaldispersion=gd3 opt scrf=(smd,solvent=ch2cl2,read)\\title\\0,1\P,-0.8666742064,-0.2661341712,-1.342714654\O,-2.228260908,0.6711423586,-1.0780595541\O,0.2835149739,0.6179150312,-0.4582165632\O,-0.6113217344,-0.2449191616,-2.8209800844\O,-0.9780117878,-1.5636955413,-0.542077618\C,-1.7606525409,2.1049925544,0.7673429042\C,-2.5070104591,1.0633139631,0.2171163662\C,-3.5825646284,0.4168107833,0.9026200379\C,-3.8595630309,0.8340226907,2.1983767132\H,-4.6923693633,0.379136014,2.7445002959\C,-3.0745444495,1.8261627066,2.8541507963\C,-1.9968056204,2.4691563871,2.1416597592\C,-1.1868753773,3.4113350642,2.8454786668\H,-0.341970981,3.877538427,2.3305104962\C,-1.4464238813,3.7274205803,4.1712667741\H,-0.8063887998,4.447714983

6,4.6927485364\C,-2.5307395649,3.1203548827,4.8603876571\H,-2.72929205
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\H,-4.1518833991,1.6976465107,4.7393603065\C,-0.7034719135,2.765732506
2,-0.0510151\C,0.3395821179,1.992809948,-0.5750588946\C,1.5258757113,2
.5812266144,-1.1210534007\C,1.5490331233,3.9592995009,-1.2935851041\H,
2.4535291094,4.4345087762,-1.6884634634\C,0.4425464218,4.7829772844,-0
.9366585336\C,-0.6985561907,4.1858667321,-0.2877940107\C,-1.7929175198
,5.0306738517,0.0702559695\H,-2.67774469,4.5880935981,0.5378447147\C,-
1.7550542568,6.3940896687,-0.1822824703\H,-2.6107023605,7.0209760655,0
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,8.0626319608,-0.990363212\C,0.454839415,6.190665401,-1.1716747248\H,1
.3322439706,6.6323679057,-1.6578870368\C,5.3389500435,-2.117706459,3.6
802260823\C,5.2089195836,-1.9076611953,2.2879440172\H,6.1035079044,-1.
7170082251,1.6845789908\C,3.9610934455,-1.9262091514,1.6679631284\H,3.
8908974061,-1.7275602517,0.5958046353\C,2.7849421325,-2.1392543665,2.4
286485494\C,2.9037903793,-2.3155558457,3.8249514255\H,2.0096594244,-2.
4684880348,4.4369973806\C,4.1642466048,-2.3246309328,4.4321206743\H,4.
2380085108,-2.4858309934,5.5132255376\C,1.4598465471,-2.0418320877,1.7
983890045\C,0.3308507063,-1.389465357,2.5398858986\H,-0.4878326563,-1.
1301152915,1.8531076782\H,0.679914019,-0.496636011,3.0798660524\H,-0.0
546466985,-2.1038551209,3.292140373\N,1.1994282264,-2.4662091096,0.582
5252286\H,0.2652864783,-2.1233266232,0.1474088819\C,1.970631779,-3.288
8276311,-0.2918389809\C,1.9181656231,-3.0021722735,-1.6688927316\H,1.3
297674146,-2.1546670529,-2.0309672002\C,2.6243346155,-3.8117827254,-2.
5681205444\H,2.5924931884,-3.5785766426,-3.6372975408\C,3.3660311224,-
4.9078544196,-2.1025060599\C,3.3911200584,-5.2021590218,-0.7281956395\
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3,0.1824500543\H,2.6975530431,-4.6391822922,1.2496594222\C,2.764493058
,1.7506300211,-1.3027970175\C,3.0310467209,1.0532188807,-2.5112882581\
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0.3094164287,-0.8719003052\C,-5.1564404493,-2.9573747169,0.0692826119\
C,-6.0140745464,-1.3135938804,-1.4643563587\C,-6.0027064996,-2.6411022
298,-1.0079924877\H,-5.1213163642,-3.9903131823,0.4344443563\H,-6.6667
434467,-1.0526068737,-2.3068252938\H,3.9174152507,-5.538016616,-2.8080
863755\C,6.6994843841,-2.1051899547,4.3307906051\H,7.1893568805,-1.123
3194194,4.1923610781\H,6.6367753526,-2.3119051351,5.411600465\H,7.3615
682601,-2.8599431492,3.8678204359\C,-5.3268765801,1.1188303948,-1.4107
206568\H,-4.6209272777,1.7485329655,-0.8445297121\C,-3.4188797981,-2.4
331847897,1.8307013984\C,-6.8775953678,-3.7038332134,-1.6668078497\H,-
7.4269078347,-3.206382011,-2.4881074634\C,-4.2130400127,-2.7154763689,
3.1232426798\H,-3.5281092926,-2.9837042653,3.9491325719\H,-4.800494984
4,-1.835741664,3.4395908561\H,-4.9166663105,-3.5567516361,2.9802320506
\C,-7.92028158,-4.2698387234,-0.681112617\H,-7.4302370126,-4.790623054
,0.1623544279\H,-8.5523512757,-3.4659909218,-0.262988762\H,-8.58074547
88,-4.997409793,-1.1877237796\C,-6.029683384,-4.8331472569,-2.28689769
49\H,-6.6745454676,-5.5609270016,-2.8130012685\H,-5.3003338211,-4.4316
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9196225526,1.2004509896,-2.8959610226\H,-5.6177880777,0.6344728565,-3.
5399488527\H,-4.926265175,2.2517116933,-3.2385219297\H,-3.9032069556,0
.7979479098,-3.0434547162\C,-6.7347947371,1.7040430798,-1.1742011297\H
,-6.7791371008,2.7556141457,-1.5128117721\H,-7.5069515725,1.1385194758
,-1.7277803911\H,-6.9990057878,1.6787212405,-0.1014808265\C,6.35206396

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74\C,2.1077415772,1.2184744409,-3.7180152225\H,1.0870885864,1.36713827
28,-3.3264509561\C,3.4164963386,2.4141771849,1.1014431475\H,2.78387280
9,3.2869269445,0.8660790448\C,5.9982337363,-2.197373404,-1.8674767303\
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,-1.0752241592\H,5.4856881565,-2.3397572528,-2.8358499314\C,7.30705044
78,-0.1929433336,-2.7303433408\H,6.837458529,-0.2511241183,-3.72949088
98\H,7.5855865358,0.8602326507,-2.5468064971\H,8.2346858963,-0.7937964
147,-2.7595112647\C,2.6164259544,1.5252583564,2.0775184946\H,1.7161850
186,1.1148307047,1.5925847961\H,3.2306768635,0.6759637655,2.4247232425
\H,2.297515826,2.1040145105,2.9637739316\C,4.6935991293,2.9501719807,1
.7720570356\H,5.2884063058,3.56816464,1.0754835773\H,4.4274158219,3.57
702598,2.642298541\H,5.3408650855,2.13425425,2.1426792569\C,2.50525096
24,2.4735300271,-4.5261997399\H,2.4768479419,3.3842346592,-3.903548186
5\H,3.5297116137,2.3717245103,-4.9308546939\H,1.8137205523,2.621290717
5,-5.3762464913\C,2.0537691209,-0.0142593386,-4.6357654334\H,1.2714940
261,0.1256694587,-5.4026609501\H,3.0095928742,-0.1791567368,-5.1673483
656\H,1.8047826098,-0.9258105236,-4.068518974\C,-2.5566783942,-3.65096
15014,1.440176736\H,-3.1713333221,-4.5599846864,1.305945828\H,-2.00945
30371,-3.4515622957,0.5050766734\H,-1.8198041371,-3.868545605,2.235277
3738\H,-2.73023371,-1.5974411353,2.0361029773\\Version=ES64L-G09RevD.0
1\State=1-A\HF=-3216.1212309\RMSD=3.633e-09\RMSF=3.332e-06\Dipole=4.17
42766,-2.23304,4.5535374\Quadrupole=7.4528551,-0.3721628,-7.0806923,-1
7.4299997,7.6444593,-5.7409684\PG=C01 [X(C65H72N1O4P1)]\\@

Solution Phase pome-ketimine/TRIP

E-configuration

E-2b/1c (Type I; conf0)
1\1\GINC-LOGIN\FOpt\RTPSSTPSS\def2SVP/W06\C65H72N1O5P1\JHIOE\05-Nov-20
15\0\\#p tpsstpss/def2svp/w06 densityfit empiricaldispersion=gd3 opt s
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,-1.3308205849\O,-1.3291085046,0.4478853205,-1.6004119637\O,0.83806249
78,0.5116515464,-0.2163146518\O,0.7492074399,-0.570116471,-2.648599808
8\O,-0.3033291775,-1.7069841789,-0.4793752761\C,-1.3621036321,2.264837
2686,-0.0363916456\C,-1.9698806537,1.1338772953,-0.5924995979\C,-3.292
076083,0.7109877254,-0.2426554307\C,-3.9863988713,1.4574051261,0.70079
66887\H,-5.0112851524,1.174122105,0.9626552543\C,-3.3947559478,2.57083
99291,1.3618884465\C,-2.0476222054,2.9599378849,1.0268406493\C,-1.4423
518988,4.007215537,1.7865212907\H,-0.4032666239,4.2817161408,1.5846217
757\C,-2.1463027287,4.6712377021,2.7805726758\H,-1.6561625971,5.466522
3696,3.3528787765\C,-3.4950671994,4.3266339073,3.0653452454\H,-4.04413
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S50

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S51

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E-2b/1c (Type I; conf1)
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E-2b/1c (Type I; conf2)
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S54

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E-2b/1c (Type II; conf0)
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S56

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E-2b/1c (Type II; conf1)
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E-2b/1c (Type II; conf2)

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,2.6194831,0.72134524,-4.2806874641\H,2.016436245,1.0325027641,-5.1537
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,5.021519\Quadrupole=14.0891295,-4.2111557,-9.8779737,-33.2547574,5.06
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Z-configuration

Z-2b/1c (Type II; conf0)
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it opt empiricaldispersion=gd3\\title\\0,1\P,-0.9261223555,0.19609813,
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9,0.8954650388,-0.5284543175\O,-0.7653669453,0.6780466194,-3.022853968
6\O,-0.8744160605,-1.2814328668,-1.2278438927\C,-1.9259670485,1.751922
6763,1.1311447573\C,-2.6030387551,0.8488946469,0.3106033542\C,-3.59003
54827,-0.0670887021,0.7928195463\C,-3.8629787638,-0.0567367846,2.15436
97071\H,-4.6338996915,-0.7223402896,2.5552293662\C,-3.1383708457,0.770
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26\H,-4.1244755706,-0.0020483872,4.8384183796\C,-0.9662730377,2.720240
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9755,3.0790448504,-0.6167944359\C,1.1033192381,4.4420262947,-0.3719846
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S62

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7\C,1.6783295522,1.7152684653,-4.744444104\H,0.8363133478,1.998535035,
-5.4007669182\H,2.6017970402,1.7711688939,-5.3501345886\H,1.51878134,0
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,-2.6495230959,-4.9238245025,-0.1432089348\H,-1.6309857188,-3.55524359
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Z-2b/1c (Type II; conf1)
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it opt empiricaldispersion=gd3\\title\\0,1\P,-0.9271628176,0.149049036
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1479,0.5284282789\C,0.128971611,2.1918887593,-0.2494244974\C,1.2162786
321,3.0342817659,-0.6477249086\C,1.1076047561,4.3972342248,-0.40473352
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\H,-5.4387647409,-3.3479600909,-4.4328521701\H,-7.0431264912,-4.081409
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,1.651292118,1.6072452713,-4.7616828437\H,0.7947874383,1.8664263855,-5
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,-2.2538529695,1.1140513458\O,7.3784156257,-3.6327199418,1.4625051097\
C,8.3343425186,-4.4602226994,0.7793347088\H,9.2521821273,-4.4133402905
,1.38318441\H,7.9830720409,-5.5062181209,0.7193474467\H,8.5372659539,-
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1824,8.2564397\PG=C01 [X(C65H72N1O5P1)]\\@

Z-2b/1c (Type II; conf2)
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it opt empiricaldispersion=gd3\\title\\0,1\P,-0.9068333922,0.328706629
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842\O,-1.0126952254,-1.1832266103,-1.4169178221\C,-1.6718568059,1.6408
131612,1.3367260437\C,-2.4661598658,0.9426767093,0.4241078553\C,-3.568
2690727,0.1172018741,0.8104532155\C,-3.8417832267,0.0006210262,2.16652
92609\H,-4.6986959326,-0.5963733976,2.4944762144\C,-3.0160684563,0.610

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79\C,-1.2715402502,1.6834700544,5.1021039719\H,-0.5833106598,2.0752501
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7\H,-4.1155398287,-0.2140434864,4.8396710574\C,-0.5857479661,2.5370031
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17,2.7474281082,-0.2944061254\C,1.7334017387,4.0397178508,0.1944280132
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7\H,-0.4093717074,-0.8033508368,1.6632641797\C,-0.5937030682,-2.153261
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6913,1.5019447175\H,2.8198603224,0.5520272099,3.0020844892\H,1.9465529
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\H,2.4534540609,4.9272987046,-2.3433639062\H,3.217976477,4.5371653131,
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,2.4554764883,-4.6221415564\H,0.6352324726,3.0299733389,-5.0714713053\
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\Quadrupole=20.9377523,2.9018675,-23.8396198,-31.1525148,-9.9958615,5.
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Z-2b/1c (Type II; conf3)
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fit opt empiricaldispersion=gd3\\title\\0,1\P,-0.9735243887,-0.0259209
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64755\C,-1.6123193494,2.883758559,4.5497790661\H,-0.9837789906,3.51866
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81\H,-4.234190922,0.6850593301,4.7797629117\C,-0.9161531007,2.71852132
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S67

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02308731,-1.3069696258\C,5.7057759084,-3.7397485719,0.009624472\H,6.40
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487332306,-2.0860524255,-2.3402877295\N,1.0290507495,-2.3063384177,0.3
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,-4.8932205995,-5.2048278865,-2.7806514266\C,-5.1216824327,1.417716501
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0121,-1.2317196255\H,-7.6857888974,0.9023882843,-1.7169567741\H,-7.232
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.1165016162,2.0793860997,2.4164758263\C,2.395605571,3.2087587121,-4.23
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83154137,-4.6407779286\H,1.7048282142,3.4553442922,-5.0579822493\C,1.9
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,8.4127997269,-3.6803620615,0.9094757362\H,9.3415324404,-3.4790165064,
1.4627912475\H,8.2037302999,-4.7652913056,0.9220970529\H,8.5170061449,
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.1739354\Quadrupole=23.1874151,2.8968696,-26.0842847,-32.9811064,-7.99
49956,5.6227919\PG=C01 [X(C65H72N1O5P1)]\\@

Z-2b/1c (Type II; conf4)
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it opt empiricaldispersion=gd3\\title\\0,1\P,-0.9027796945,0.193423662
8,-1.6252410398\O,-2.3356703908,0.8608054359,-1.0646908644\O,0.1933699
987,0.8983140258,-0.5321126273\O,-0.7360856101,0.6802679119,-3.0329325
202\O,-0.8433097106,-1.2843294011,-1.2429468248\C,-1.9252930339,1.7439
791973,1.1112809857\C,-2.5919824866,0.8329970557,0.2908748481\C,-3.573
311259,-0.0881870417,0.7739593779\C,-3.8464318839,-0.080238367,2.13548
02545\H,-4.6148236778,-0.7495422249,2.5352865325\C,-3.1318751994,0.755
7643535,3.0409912886\C,-2.1370575816,1.6695106329,2.5347355719\C,-1.36
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327,3.0904452218,-0.634388184\C,1.0810629882,4.4545472953,-0.402478897
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87707707,2.6566187597\C,3.9609296272,-2.355037339,1.2471826242\H,3.323
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\H,-0.2614634904,-0.5564262947,1.5434826248\C,-0.2914882815,-1.5262158
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,-3.4658836893\C,-3.6684651426,-3.7053675613,2.0117515302\H,-2.8963083
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,1.7283246139,-4.7573385342\H,0.877728081,2.0332792579,-5.4266106669\H
,2.635644662,1.7626982568,-5.3490746183\H,1.5110619455,0.687483757,-4.
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.9387554053,-0.2531329107\H,-1.6592288024,-3.5589210369,-0.8459816195\
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72,1.157389924\O,7.3426473473,-3.8154561312,1.4688926624\C,7.880668611
4,-3.1916416894,2.6460526499\H,8.9045863416,-3.5804533029,2.7455318408
\H,7.9116610808,-2.0927791403,2.5333621188\H,7.2929576661,-3.461532127
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8\PG=C01 [X(C65H72N1O5P1)]\\@

Z-2b/1c (Type II; conf5)
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yfit opt empiricaldispersion=gd3\\title\\0,1\P,-0.9277175602,0.1762338
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32234\O,-0.836372951,-1.3073544335,-1.2481015984\C,-1.891108086,1.6679
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3\H,-3.9543347012,-0.1775680881,4.9320619164\C,-0.968172349,2.66446527
99,0.5766655106\C,0.0980179911,2.2165338746,-0.210954724\C,1.168197656
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,0.9158402284\C,5.3115606625,-2.5809297915,1.6126849743\H,5.648478754,
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\H,6.3713397918,-4.7763375242,-0.7978466592\C,2.246068278,-2.592657206
9,-0.6208876064\C,2.0944822761,-2.4934707671,-2.1114631744\H,1.0921222
689,-2.1334667393,-2.3849888031\H,2.2510286347,-3.4882719643,-2.566714
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20709,2.6789846971,-3.5329595915\H,0.6648261671,2.6224596976,-3.053504
576\C,3.2301949831,2.4325921435,1.3435970841\H,2.4768039827,3.23482899
04,1.4177265477\C,7.4215684038,1.469511996,-2.0044788566\H,8.345918604
1,1.0152746161,-2.4062142217\H,7.3462797675,2.4991008197,-2.3981233871
\H,7.5295981229,1.5325172612,-0.9059215403\C,6.3049546153,-0.812473373
5,-1.8675435574\H,6.3311658185,-0.8308743522,-0.7628371503\H,5.4468085
867,-1.4255425321,-2.19267881\H,7.2291101148,-1.2955532585,-2.23462370
95\C,2.6410710717,1.1947205555,2.0504307827\H,1.7772299542,0.795927063
5,1.4963844547\H,3.3994140795,0.3954263095,2.1215033382\H,2.3098038137
,1.44347223,3.0750981069\C,4.493634881,2.9308087248,2.0687599069\H,4.9
271085299,3.8145712161,1.5666428053\H,4.244507018,3.2156184257,3.10711
64867\H,5.2750771488,2.1507554251,2.1216556916\C,1.9093580473,4.144814
1454,-3.9493795194\H,1.8844143574,4.822603677,-3.0783979298\H,2.898147
1472,4.2516189597,-4.4338905966\H,1.1385847922,4.4832676114,-4.6664359
579\C,1.601849057,1.7639888695,-4.7678597775\H,0.7535144381,2.05633938
24,-5.4120842894\H,2.5198530609,1.8347241188,-5.3803280203\H,1.4484630
657,0.7125637797,-4.4739666157\C,-2.006454247,-4.0836783842,0.00245629
33\H,-2.5516502094,-5.002331016,-0.2824621782\H,-1.6226868873,-3.60122
44157,-0.9104284074\H,-1.1442321143,-4.3915326722,0.6208612144\H,-2.25
23604731,-2.2859465565,1.1422505927\O,7.4200650096,-3.7782708535,1.293
2663442\C,7.9690763571,-3.1637477052,2.4702621252\H,8.9946115349,-3.55
15703399,2.5558282245\H,7.9970277167,-2.0638560465,2.3669397425\H,7.39
08921319,-3.4420483108,3.369929011\\Version=ES64L-G09RevD.01\State=1-A
\HF=-3291.2881191\RMSD=4.768e-09\RMSF=4.093e-06\Dipole=5.1407385,-3.12
65767,3.9850297\Quadrupole=17.8829732,-2.5039966,-15.3789766,-21.13243
59,5.4981991,2.7032137\PG=C01 [X(C65H72N1O5P1)]\\@

Z-2b/1c (Type II; conf6)
1\1\GINC-LOGIN\FOpt\RTPSSTPSS\def2SVP/W06\C65H72N1O5P1\JHIOE\27-Jan-20
16\0\\#p scrf=(smd,solvent=ch2cl2,read) rtpsstpss/def2svp/w06 densityf
it opt empiricaldispersion=gd3\\title\\0,1\P,-0.8984572186,0.329415864
9,-1.5726115685\O,-2.2374579507,1.0841843325,-0.9048140787\O,0.2711141
111,0.7771222437,-0.4283272707\O,-0.6966408516,0.9558366787,-2.9189949
126\O,-0.9762490822,-1.1827563641,-1.3630971425\C,-1.7350015878,1.6392
098633,1.3636714806\C,-2.500673828,0.9235197139,0.4394091446\C,-3.5914
627861,0.074951374,0.8080851553\C,-3.8885432058,-0.0404768404,2.159324
8922\H,-4.7373056199,-0.6557334645,2.4744700459\C,-3.0931008481,0.5887
280716,3.1594747723\C,-1.978975495,1.4179455244,2.7690281968\C,-1.1382
213586,1.9423748269,3.7971307419\H,-0.2623097931,2.5348218142,3.519020
5888\C,-1.4048466893,1.696900463,5.1363549516\H,-0.7379452576,2.102802
6471,5.9048663315\C,-2.5301409701,0.9187609515,5.5194386119\H,-2.73423
01773,0.7387192542,6.5805177293\C,-3.3533316363,0.373651857,4.54676401
58\H,-4.2095537369,-0.2508146209,4.8259456066\C,-0.6586171308,2.555356
9554,0.8890763982\C,0.3469282319,2.070083476,0.0442984617\C,1.53675409
3,2.8131811795,-0.2425304622\C,1.6342576661,4.1061792825,0.2504305148\
H,2.5409401802,4.6886732,0.0581259676\C,0.5804910013,4.7073092155,0.99
77991099\C,-0.5902910124,3.9300805956,1.3188077596\C,-1.6479799821,4.5
685327323,2.0351932518\H,-2.5586500707,4.0037834791,2.255503236\C,-1.5
42993512,5.8917366713,2.4382019088\H,-2.3721103675,6.3619972489,2.9783

742541\C,-0.3736933348,6.6451118602,2.1490175383\H,-0.3012580359,7.687831295,2.4770380403\C,0.6633563724,6.0624902515,1.4377338764\H,1.5634218517,6.6376822759,1.1921516316\C,5.8348358995,-3.5324405844,1.2589441486\C,4.8741470537,-2.789209739,1.9849062942\H,5.0733757111,-2.4546986226,3.0055853992\C,3.6559530716,-2.4674920882,1.3890239073\H,2.937603734,-1.8774524873,1.9614230824\C,3.3609906545,-2.8429776013,0.0549264424\C,4.3481935094,-3.5649714919,-0.6663592264\H,4.1583467892,-3.8762993904,-1.6970791811\C,5.553775278,-3.9199692246,-0.0725821005\H,6.3054340637,-4.4940969351,-0.6223084808\C,2.1179547528,-2.4231120941,-0.6023730866\C,2.1398495606,-2.0281650987,-2.0499518144\H,1.1249729284,-1.8348946794,-2.4249053434\H,2.6131652619,-2.8161131138,-2.6588047335\H,2.7552882025,-1.1164967714,-2.1626018179\N,0.9663470861,-2.2912065921,0.0217708263\H,0.1657396096,-1.8271898667,-0.541540401\C,0.5950900198,-2.67420852,1.3465679661\C,-0.1566727872,-1.7582257961,2.1026508965\H,-0.4017954808,-0.7814655272,1.6772719704\C,-0.5747669351,-2.1108105926,3.3934139503\H,-1.1508350829,-1.3926930883,3.9852891287\C,-0.263096482,-3.3754497928,3.9152363673\C,0.463968624,-4.2953432022,3.1390735526\H,0.690897823,-5.2910919277,3.534501204\C,0.8945161962,-3.9526206234,1.8518919706\H,1.4487469928,-4.667646306,1.2374084603\C,2.6653292911,2.1712278354,-0.996237015\C,2.7218068894,2.2993637308,-2.4117114927\C,3.6769239828,1.444572546,-0.3068857641\C,3.7812898432,1.6924210854,-3.1118811356\C,4.707270243,0.8472539295,-1.0610618719\C,4.784059764,0.9572650857,-2.459764749\H,3.8311885709,1.7936244674,-4.2016711176\H,5.4753784481,0.277536537,-0.5230133552\C,-4.3747119356,-0.6553441072,-0.2403500544\C,-4.2935824807,-2.0746281034,-0.3304866465\C,-5.204587734,0.0641487819,-1.1419347939\C,-5.0691719502,-2.7394810919,-1.2964488356\C,-5.9523380349,-0.6492957216,-2.0982080673\C,-5.9056968757,-2.0492092434,-2.1916273423\H,-5.0084181556,-3.8320543353,-1.3594739173\H,-6.5957204787,-0.0953821364,-2.7932312657\H,-0.594794413,-3.6501745012,4.9221022283\C,-5.3358681297,1.5874621207,-1.0902981102\H,-4.6622342046,1.9610316595,-0.3008324261\C,-3.3776326223,-2.8968224951,0.5788122135\C,-6.7295398523,-2.7940686519,-3.2387823433\H,-7.2744164672,-2.0301747055,-3.8251482733\C,-4.1784577169,-3.6277676967,1.6765552839\H,-3.4974406332,-4.1760032704,2.3535448551\H,-4.7717536512,-2.9239987618,2.2858890752\H,-4.8781484445,-4.35984538,1.2318301251\C,-7.7774226407,-3.7181275077,-2.5845399959\H,-7.2916497541,-4.5118942307,-1.9871630536\H,-8.4475540055,-3.1513341135,-1.9135715085\H,-8.3996751539,-4.20945156,-3.3552369904\C,-5.8308722054,-3.5806241087,-4.2151650428\H,-6.438637363,-4.0571406923,-5.0061587884\H,-5.0929869614,-2.9174415036,-4.7007154704\H,-5.2753560439,-4.3799065773,-3.6908881026\C,-4.896884464,2.2435864619,-2.4154783957\H,-5.5629939977,1.955100922,-3.2494343648\H,-4.9289900844,3.3454313,-2.3280176823\H,-3.8660693508,1.9491947431,-2.6744972225\C,-6.7670374209,2.0108546118,-0.698205835\H,-6.8341264159,3.1106252426,-0.6068529971\H,-7.5051108417,1.6892857839,-1.4559828564\H,-7.0612788174,1.5689028299,0.2708746329\C,5.9200304739,0.310567347,-3.2481146659\H,5.7484944831,0.549714881,-4.3145675625\C,1.6904954231,3.1405203522,-3.1670035871\H,0.7532496351,3.1034186028,-2.5858313181\C,3.8048194851,1.3172511414,1.2195742727\H,4.5052567751,0.4749062923,1.3684240878\C,7.2909170331,0.8959835347,-2.8505933678\H,8.0941786995,0.4641604651,-3.4756114551\H,7.3099327266,1.9932250214,-2.9771815712\H,7.5289902191,0.6720299097,-1.7942543589\C,5.9129371028,-1.2245311236,-3.1044902816\H,6.0807288821,-1.5274410297,-2.0554201362\H,4.9488992359,-1.6511069134,-3.4317795036\H,6.7134565439,-1.6773017083,-3.7179321916\C,4.4908579296,2.5656991222,1.8180839519\H,5.4504830705,2.7759046291,1.313047979\H,3.8493552207,3.4588093557,1.7173480541\H,4.6947058162,2.4136425091,2.8943309856\C,2.5296145919,0.9616133875,2.0099919061\H,1.9236850854,0.206273

0859,1.485545802\H,2.8115189685,0.5518791811,2.9968579432\H,1.89152859
18,1.8409305184,2.1927811071\C,2.1545238436,4.6118569101,-3.2489998326
\H,2.3278595686,5.0435870008,-2.2486722118\H,3.0989258305,4.6903852423
,-3.8196768012\H,1.3936794773,5.2304734692,-3.7601060739\C,1.366302581
9,2.6049026163,-4.5726514441\H,0.5156223814,3.1684289299,-4.9966005996
\H,2.2173617059,2.723308256,-5.2685855852\H,1.0751472762,1.5437690125,
-4.5297617156\C,-2.5081152428,-3.8939898815,-0.2124270168\H,-3.1163502
616,-4.6961947977,-0.6694525022\H,-1.9521847771,-3.3731042304,-1.00856
13625\H,-1.7796290307,-4.3767566348,0.4636237378\H,-2.6897276595,-2.19
32096361,1.074819889\O,7.0352496199,-3.9089841627,1.7448082454\C,7.391
1466747,-3.5498168181,3.0897692779\H,8.3930038646,-3.9724227544,3.2543
462234\H,7.4280472367,-2.4518535016,3.210896135\H,6.6816954527,-3.9839
307632,3.817330076\\Version=ES64L-G09RevD.01\State=1-A\HF=-3291.287353
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drupole=13.200669,-2.8185636,-10.3821054,-19.448881,5.7237929,-0.88224
17\PG=C01 [X(C65H72N1O5P1)]\\@

Z-2b/1c (Type II; conf7)
1\1\GINC-LOGIN\FOpt\RTPSSTPSS\def2SVP\W06\C65H72N1O5P1\JHIOE\26-Jan-20
16\0\\#p scrf=(smd,solvent=ch2cl2,read) rtpsstpss/def2svp/w06 densityf
it opt empiricaldispersion=gd3\\title\\0,1\P,-0.9553674136,0.025676235
5,-1.6351475043\O,-2.3652821578,0.8001943695,-1.1645850734\O,0.1541844
415,0.7664286457,-0.5779634688\O,-0.7447544319,0.3923245787,-3.0737253
015\O,-0.9620640206,-1.4184092135,-1.1360768006\C,-1.9454870234,1.9298
985633,0.8911734588\C,-2.6444189851,0.9557030278,0.1765756327\C,-3.680
3946367,0.1525759057,0.7482326643\C,-3.9741530895,0.3446716109,2.09228
14735\H,-4.7764740339,-0.2383330884,2.5560244039\C,-3.2305900469,1.250
3028823,2.9028117758\C,-2.1841927783,2.0458099322,2.3080529136\C,-1.39
58590318,2.8742547874,3.1630110973\H,-0.5726696234,3.4534204401,2.7351
182313\C,-1.6433634862,2.9356527684,4.5267601265\H,-1.0161610051,3.569
0763596,5.1636555075\C,-2.6972606486,2.1785192437,5.1053122779\H,-2.88
61214159,2.2399759007,6.1826125839\C,-3.4717425475,1.3518124837,4.3064
666051\H,-4.2734192282,0.7458378918,4.7438031387\C,-0.9203264077,2.764
9755496,0.2022685249\C,0.1576862094,2.1392985293,-0.4330733986\C,1.333
2268781,2.8564614093,-0.8278963852\C,1.3042779864,4.2429559378,-0.7591
012634\H,2.1962005391,4.8137308477,-1.0395851966\C,0.1565206281,4.9481
878791,-0.2922150897\C,-0.9669696298,4.2040928714,0.2223270961\C,-2.09
59754184,4.9297034573,0.709150013\H,-2.9646298844,4.3767122591,1.07957
58221\C,-2.1107799914,6.3167877112,0.7013321684\H,-2.9920351658,6.8525
629009,1.0710791798\C,-0.9959517379,7.0484729096,0.210693799\H,-1.0188
823201,8.1437430654,0.2131216699\C,0.1126546255,6.3744589285,-0.277834
6638\H,0.9757570353,6.9277199458,-0.6653538508\C,6.1118896873,-3.01056
53247,1.2364400095\C,5.1951323801,-2.1146055862,1.8347719517\H,5.49598
87777,-1.4668977221,2.661277635\C,3.8940198864,-2.0327492536,1.3441280
05\H,3.210006806,-1.3106507093,1.7939905816\C,3.4658402772,-2.81122420
59,0.2422476412\C,4.4042979476,-3.6932562023,-0.35619944\H,4.112737577
8,-4.3069271928,-1.2131664402\C,5.6955558581,-3.8093876281,0.144387066
6\H,6.4161703726,-4.4968694811,-0.3080545102\C,2.1485175708,-2.5977562
826,-0.3608220085\C,2.0044662386,-2.684575377,-1.8525999775\H,0.984879
7764,-2.4200474674,-2.1678097557\H,2.226742266,-3.7146149725,-2.185119
6746\H,2.7370188862,-2.0167609909,-2.3373443575\N,1.0648751786,-2.2651
996835,0.3120444191\H,0.2285429679,-1.9319770722,-0.2848375276\C,0.794
9772174,-2.2617565603,1.7125637796\C,-0.0501630765,-1.248482377,2.2018
979575\H,-0.4239490747,-0.4814079664,1.5188206814\C,-0.4010800964,-1.2
345190378,3.5584058327\H,-1.0536186703,-0.4398426089,3.9339847883\C,0.
0717283413,-2.2357378655,4.4200797212\C,0.8938362804,-3.2600841317,3.9

S74

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Z-2b/1c (Type I; conf0)

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fit opt empiricaldispersion=gd3\\title\\0,1\P,-1.0989947322,0.06897357
95,-1.4566957374\O,-2.4697724476,0.7573154192,-0.7813581282\O,0.102494
4608,0.800592056,-0.5005139655\O,-1.0671082421,0.5202478672,-2.8862735
872\O,-0.9862312422,-1.3958054932,-1.0373181975\C,-1.8498205169,1.7101
524753,1.3140207848\C,-2.6039303247,0.7844788398,0.5913110906\C,-3.561
654199,-0.0909208889,1.1932471593\C,-3.6949631111,-0.0436917461,2.5752
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802242,2.977344861,-0.7448840149\C,1.0304297902,4.3473929947,-0.534409
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,0.6035458513,6.9874262121,-0.1233738375\C,5.4519578001,-2.8757133725,
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139616\H,-4.5288848501,-4.5970202662,2.2060084618\C,-7.7669533733,-4.5
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,-4.1656489734\H,1.7467830244,4.6492650712,-3.3209643706\H,2.640407415
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,1.2014562541,1.5530920647,-4.8709388409\H,0.3387454039,1.8842318778,-
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Z-2b/1c (Type I; conf1)
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it opt empiricaldispersion=gd3\\title\\0,1\P,-1.0915156623,0.049404508
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\O,-0.947066825,-1.4232334545,-1.0668459979\C,-1.8227435105,1.60506225
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Z-2b/1c (Type I; conf2)
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Z-2b/1c (Type I; conf3)
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4919611987\C,-6.9645554483,1.5879425499,-0.1652981283\H,-7.0897441698,
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3,-4.0859804885\H,1.8425689918,4.6684700743,-3.229192659\H,2.759921677
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111247,2.730466031\H,8.4458846251,-3.5088549692,3.6075083294\H,7.79079
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,-1.9982115,-0.658707\PG=C01 [X(C65H72N1O5P1)]\\@

Z-2b/1c (Type I; conf4)
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it opt empiricaldispersion=gd3\\title\\0,1\P,-1.099150696,0.0914260875
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,-0.9990504288,-1.3798773063,-1.0028583238\C,-1.8372147921,1.661167503
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8\C,-1.156800117,2.2364555148,5.0867025113\H,-0.4811295251,2.8158843504,5.7255142219\C,-2.1240153486,1.3799801052,5.6778408214\H,-2.1982620117,1.3115311787,6.7686657915\C,-2.9591782347,0.6216856931,4.8722409957\H,-3.6964597676,-0.0568491597,5.3165281399\C,-0.9330269266,2.6245289007,0.7196395315\C,0.0670428431,2.1444242772,-0.1335243587\C,1.134146254,2.9743342612,-0.6036929928\C,1.0708748503,4.3353867769,-0.3360233192\H,1.8874138524,4.9866181022,-0.666074137\C,-0.0160921203,4.9095692415,0.3848933246\C,-1.0306799234,4.0454489074,0.9359385118\C,-2.1111929533,4.64225123,1.6541027223\H,-2.9063518617,4.0028036484,2.0495415028\C,-2.1749249467,6.0156564407,1.8379949287\H,-3.0188225681,6.451565492,2.3840432239\C,-1.1602994014,6.8627927465,1.3166516065\H,-1.2199603148,7.945440177,1.4729970932\C,-0.1052934207,6.3174528116,0.6017855524\H,0.6772990709,6.9614693644,0.184461064\C,5.5452123179,-3.132571669,2.6549786349\C,5.4237882499,-2.5025200351,1.3935599387\H,6.3062766334,-2.1746299314,0.8397389647\C,4.1601028498,-2.2825534465,0.8500739979\H,4.0912823203,-1.7649514314,-0.1095668865\C,2.9820034559,-2.6578126042,1.5429990276\C,3.1221581333,-3.2504141866,2.8263225738\H,2.2352243585,-3.5399926054,3.3970574459\C,4.377835212,-3.5014308106,3.3657910828\H,4.4875873168,-3.9788940263,4.3440106307\C,1.6508852626,-2.3430127563,1.0239023931\C,0.5252337322,-2.0433870436,1.973321672\H,-0.3308110051,-1.6171688314,1.4307015603\H,0.857534795,-1.3516312373,2.7632996603\H,0.1988853105,-2.9789704843,2.4633874011\N,1.3566660974,-2.262434666,-0.2560581583\H,0.374588061,-1.8834468243,-0.5088485081\C,2.1201840336,-2.6226178554,-1.4091470675\C,2.1594106376,-1.7058125524,-2.4740618939\H,1.6871050546,-0.7253353772,-2.3695699048\C,2.8305759844,-2.0515356018,-3.6545027172\H,2.8672106536,-1.333876246,-4.4802526785\C,3.4563582504,-3.3017796512,-3.7717557163\C,3.4052101172,-4.214457689,-2.7035122926\H,3.8820070892,-5.1960323422,-2.795526271\C,2.7324064007,-3.8846829752,-1.5206083203\H,2.6731155856,-4.5955903905,-0.6914631603\C,2.3559740766,2.343793848,-1.2056597943\C,2.4679652735,2.1284674054,-2.6023969491\C,3.4136281647,1.9613533317,-0.3307726184\C,3.6317003986,1.5103264965,-3.0988498267\C,4.5469133037,1.3309793519,-0.8759429901\C,4.6742567795,1.0904169511,-2.2563913932\H,3.731216788,1.3426385072,-4.1768220852\H,5.3568156631,1.0251718077,-0.205148626\C,-4.385255517,-1.0143613316,0.3537375619\C,-4.2261595967,-2.4267113335,0.4030632793\C,-5.3416357101,-0.4420634858,-0.5329295759\C,-5.0401147536,-3.231413587,-0.4173425437\C,-6.1246486756,-1.2905608968,-1.3342824227\C,-5.9940420525,-2.690048331,-1.2927064609\H,-4.9215975639,-4.321130649,-0.3793317264\H,-6.8629496877,-0.8427260537,-2.0098576687\H,3.9817082013,-3.5682245509,-4.694865049\C,-5.575798464,1.0682007304,-0.6200360806\H,-4.8562870737,1.5668934167,0.05071971\C,-3.1933195816,-3.1056649087,1.3047024684\C,-6.8536168776,-3.5930535025,-2.1728620155\H,-6.5551374774,-4.6361098315,-1.9550284229\C,-3.8721872178,-3.8322944891,2.4846918676\H,-3.1139695436,-4.2742371539,3.1576125259\H,-4.4964401923,-3.1418851282,3.0790022812\H,-4.5238129917,-4.6506435367,2.1256037593\C,-6.5944898966,-3.3345049223,-3.6713797392\H,-6.89004945,-2.307761578,-3.9555426747\H,-5.5252209981,-3.4605557265,-3.918190962\H,-7.1766142451,-4.0377488559,-4.2949904458\C,-8.3524023266,-3.4534979819,-1.8359561208\H,-8.9553879517,-4.1557496173,-2.4405194229\H,-8.5431317873,-3.6684590087,-0.7691830871\H,-8.7152803529,-2.4305080966,-2.0466198987\C,-5.3227693284,1.6061236204,-2.0432925401\H,-6.0468340178,1.1903106282,-2.7682556846\H,-5.4273211335,2.7066960491,-2.0610368941\H,-4.3043660338,1.3520844568,-2.3815896734\C,-6.9871894922,1.4401331642,-0.1195031117\H,-7.1272953014,2.536703705,-0.1356261285\H,-7.7721214541,0.9902517022,-0.7550819788\H,-7.1469102439,1.0897664236,0.9161816739\C,5.9226307799,0.4288116214,-2.8350386684\H,5.7121654497,0.2200232645,-3.900978244\C,1.368886349,2.6040924681

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S84

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7\Quadrupole=22.0444871,-5.4816319,-16.5628551,-17.9904895,4.1778209,-
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Solution Phase pcf3-ketimine/TRIP

E-configuration

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E-2c/1c (Type II; conf1)

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S93

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E-2c/1c (Type II; conf2)
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3N1O4P1)]\\@

Z-configuration

Z-2c/1c (Type II; conf0)
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0.4744465438\C,0.4595217602,2.0846361358,-0.2864520299\C,1.6423910991,
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S96

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S98

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Z-2c/1c (Type II; conf2)
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9F3N1O4P1)]\\@

Z-2c/1c (Type II; conf3)
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,1.2895518277\C,5.1745507231,-2.4085746608,1.827337985\H,5.545269621,-
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S101

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\@

Z-2c/1c (Type I; conf2)
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Solution Phase pcf3-pome-ketimine/TRIP

E-configuration

E-3a/1c (Type I; conf0)
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E-3a/1c (Type I; conf4)
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,-4.2340034321\H,3.2752844323,2.7699076511,-3.9369806265\H,4.557746587
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,-4.63476272\H,4.1555832967,-0.9613367924,-3.8713046599\H,2.6867932798
,-1.4336836519,-2.949169273\C,-2.9033265689,-2.9517469387,2.4869653311
\H,-3.3166947893,-3.9771736679,2.4827698165\H,-2.0283142435,-2.9192947
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E-3a/1c (Type II; conf1)
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\C,-7.1783493575,-0.1932555868,1.8476197247\H,-7.3183378135,-1.2337975
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,2.697895053,2.8104470966,3.1708388456\H,3.5223113537,1.0098597209,1.7
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N1O5P1)]\\@

E-3a/1c (Type II; conf2)
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S122

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Z-3a/1c (Type II; conf0)

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S125

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1.5678594366\H,-1.149926025,-4.3033478093,-0.1800811908\H,-2.383655790
4,-2.3597822025,0.6388089811\F,8.2820440117,-2.1019186225,0.0563648821
\F,7.6203767101,-3.1977877128,1.8195809783\F,8.0379267884,-4.266748239
,-0.0390163359\O,0.1523814876,-3.4375451076,4.7398634952\C,-0.69353523
89,-2.6540257014,5.594544493\H,-0.7101218078,-3.1793754586,6.560801577
\H,-0.2864167387,-1.6358218602,5.7331980865\H,-1.7194062134,-2.5917513
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adrupole=-12.9666813,4.8442904,8.1223909,-2.4760274,-22.2071978,14.496
1097\PG=C01 [X(C66H71F3N1O5P1)]]\\@

Z-3a/1c (Type II; conf2)
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g-2016\0\\#p tpsstpss/def2svp/w06 densityfit empiricaldispersion=gd3 o
pt scrf=(smd,solvent=ch2cl2,read)\\title\\0,1\P,-0.7140326512,0.714272
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,1.0697187703\C,0.6239635992,2.0556605085,0.2016149568\C,1.8953976216,
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S127

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,2.8393246096,-4.2468829657\H,1.3470864917,3.5077501281,-4.6980974596\
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S128

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1 [X(C66H71F3N1O5P1)]\\@

Z-3a/1c (Type II; conf3)
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 scrf=(smd,solvent=ch2cl2,read)\\title\\0,1\P,-1.3483305331,0.54120452
3,-1.7561538493\O,-2.7754133273,1.0324568298,-1.0334829078\O,-0.221714
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,2.0752061522,2.7774882407,-0.7826181023\C,2.3555082004,2.6729919095,-
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S129

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1271013\PG=C01 [X(C66H71F3N1O5P1)]\\@

Z-3a/1c (Type I; conf0)
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pt scrf=(smd,solvent=ch2cl2,read))\\title\\0,1\P,-0.9818677008,-0.28647

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S132

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Z-3a/1c (Type I; conf2)
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56524,0.9972402681,-0.4998231984\O,-1.4838556924,0.3419441607,-2.87419
36446\O,-1.1461084039,-1.3813289567,-0.8721427573\C,-2.5678940847,1.68
88389488,1.2176101924\C,-3.134863403,0.6022327454,0.5506125798\C,-3.93
36090196,-0.3928413985,1.1971244377\C,-4.113732151,-0.2775058574,2.569
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1293327,3.327196013\C,-2.6785493519,1.7436383278,2.6537366755\C,-1.995
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22264\C,-2.1251284127,2.7274916237,4.8290780008\H,-1.5851423863,3.4775
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152744,1.7981857967,6.5780264104\C,-3.6049127517,0.802708952,4.7486370
099\H,-4.2252007272,0.0486614049,5.2465159935\C,-1.8208587034,2.723350
0186,0.4446913381\C,-0.728487986,2.3393149505,-0.3405027954\C,0.192895
9717,3.2858265306,-0.8925762134\C,-0.1134602207,4.6351237404,-0.780851
3113\H,0.5847493647,5.3803598965,-1.1765201254\C,-1.3029605861,5.08321
68617,-0.1355821096\C,-2.1659960376,4.1208520792,0.505033485\C,-3.3489
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=-12.4463736,3.1263475,9.3200261,-3.2259177,-25.3660731,-0.2278843\PG=
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Z-3a/1c (Type I; conf3)
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9903075\O,-0.8287335601,-1.5493773559,-0.5242168213\C,-2.2092256134,1.
9501111702,0.802519814\C,-2.792011198,0.7966455851,0.2756996152\C,-3.7
493078862,0.0023842917,0.9821538092\C,-4.0738386825,0.3905207738,2.276
0670735\H,-4.8201258811,-0.1803691191,2.8385432103\C,-3.4394714844,1.4
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,-5.2320270651,-1.0099003952,-0.7980274503\C,-4.7563122096,-3.59370422
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S136

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,-3.2988349548,-3.3625086695,4.1077674436\H,-4.7412104926,-2.472991214
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Z-3a/1c (Type I; conf4)
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Solution Phase pch3-pome-ketimine/TRIP

E-configuration

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S139

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S140

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7159,-1.6449238206\H,7.2605092009,-5.5805795083,-2.2692725361\H,6.9206

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E-3b/1c (Type I; conf2)
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E-3b/1c (Type I; conf3)
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S144

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36130227,-3.1703638684\H,6.3743969451,-2.640340909,-2.8804323873\H,6.6
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N1O5P1)]\\@

E-3b/1c (Type I; conf4)
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739973\H,-5.3042142637,0.5820932407,1.0805372374\C,-3.8986621282,2.201
0969549,1.4473697411\C,-2.641188419,2.7976261622,1.0663212908\C,-2.178
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13011\C,-2.9316796029,4.4633506135,2.8411477573\H,-2.5496195973,5.3243
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Quadrupole=2.8335245,-5.2604859,2.4269613,-15.9182671,-10.4039154,-11.
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E-3b/1c (Type II; conf0)
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\H,5.9336098832,-2.6560970964,1.9914952575\C,0.7820136087,-2.578524332
7,-1.0675742409\C,-0.4330785225,-1.9165767445,-0.8686531768\C,-1.69201
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G=C01 [X(C66H74N1O5P1)]\\@

E-3b/1c (Type II; conf1)
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,-5.7810842883,-3.1439865615,2.0158395452\C,-6.8824606032,-5.233237101
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 [X(C66H74N1O5P1)]\\@

E-3b/1c (Type II; conf2)
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S151

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S155

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6H74N1O5P1)]\\@

Z-3b/1c (Type II; conf2)

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S157

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Z-3b/1c (Type II; conf3)
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S162

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Z-3b/1c (Type I; conf2)
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Z-3b/1c (Type I; conf3)
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Solution Phase pno2-pome-ketimine/TRIP

E-configuration

E-3c/1c (Type I; conf0)

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E-3c/1c (Type I; conf1)
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6,-17.7547312,16.8029621\PG=C01 [X(C65H71N2O7P1)]\\@

E-3c/1c (Type II; conf1)
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E-3c/1c (Type II; conf2)
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