Relaxation Dispersion NMR to reveal fast Dynamics in Brønsted Acid Catalysis: Influence of Sterics and H-bond strength on conformations and substrate hopping

N. Lokesh, Johnny Hioe, Johannes Gramüller and Ruth M. Gschwind*

Institute for organic chemistry,
University of Regensburg, D-93053 Regensburg, Germany

E-mail : ruth.gschwind@chemie.uni-regensburg.de

Supplementary Material

Experimental data

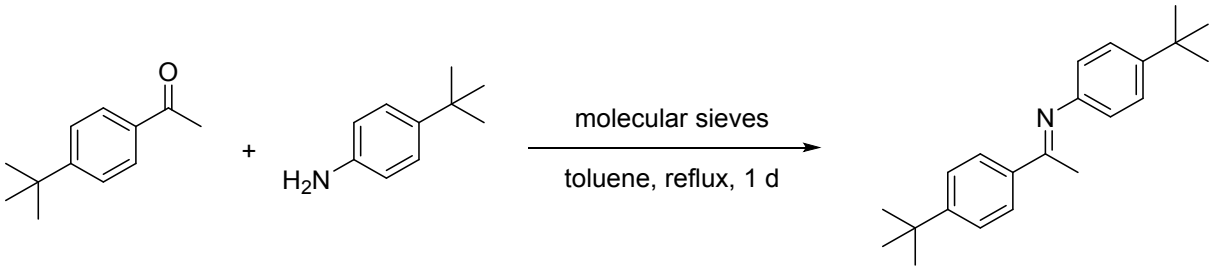
Deuterated solvents were purchased from Deutero or Sigma Aldrich. Where dry solvents were essential, CD_2Cl_2 was freshly distilled over CaH_2 and Toluene was refluxed over Na/Benzophenone under argon atmosphere. The catalysts were purchased from Sigma Aldrich or STREM chemicals.

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 Imine Substrates

The imines were prepared as described in the literature.[1–4] The toluene was used either in p.A. quality or was dried by refluxing over sodium. The ^{15}N-enriched aniline (if used) was purchased from Euriso-top GmbH and Sigma Aldrich.

(E)-N,1-bis(4-(tert-butyl)phenyl)ethan-1-imine [5]



Molecular sieves 4 Å (4 g) was weighed into a 50 mL Schlenk flask and dried with a heat gun at 350 °C for 30 min under reduced pressure. Under Argon flow, 4-(*tert*-butyl)aniline (10.0 mmol, 1.49 g, 1.60 mL, 1.0 eq) and 1-(4-(*tert*-butyl)phenyl)ethan-1-one (10.0 mmol, 1.76 g, 1.83 mL, 1.0 eq.) were added and dissolved in 20 mL anhydrous toluene. Under Argon flow, a reflux condenser was added to the setup and flushed with argon for 3 min. A drying tube filled with $CaCl_2$ was added to the setup. The solution was refluxed for 24 h. Afterward, the heating bath was removed, and the reaction mixture allowed to cool down. The orange mixture was filtrated, and the solvent was removed under reduced pressure to give an orange-yellow solid. The crude product was washed with methanol to give the product (4.76 mmol, 1.46 g, 48%) as yellow needles predominantly as its *E*-isomer (>99% determined by ^{1}H NMR).

^{1}H-NMR (400.1 MHz, CD_2Cl_2) δ_H = 7.91 (m, 2H), 7.48 (m, 2H), 7.37 (m, 2H), 6.71 (m, 2H), 2.21 (s, 3H), 1.36 (s, 9H), 1.34 ppm (s, 9H).

^{13}C-NMR {^{1}H} (100.6 MHz): δ_C = 164.8, 153.7, 149.2, 145.8, 137.0, 126.8, 125.7, 125.2, 119.0, 34.7, 34.1, 31.2, 31.0, 16.9 ppm.

HR-MS (ESI, *m/z*): found 307.2289 (M)+ (calculated for 307.2300 for C22H29N); Diff(ppm) = -1.92 ppm.

Sample preparation

Preparation of binary complexes in CD_2Cl_2

The catalyst was dried for 30 min at 150°C under reduced pressure. Ketimine and catalyst were directly weighed into a 5 mm NMR tube under an inert argon atmosphere. CD_2Cl_2 (0.6 ml; freshly destilled over CaH_2) 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/ketimine was used for all samples unlike stated otherwise. A concentration of 0.25 – 100 mM was used, as indicated specifically.

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 CPPBBO BB-1H/19F. The 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 otherwise noted. 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 ^{19}F and ^{31}P were referenced, employing $\nu(X) = \nu(TMS) \times \Xi_{reference} / 100$ % according to Harris et al.[5] The following frequency ratios and reference compounds were used: Ξ (^{19}F) = 94.094011 (CCl_3F), Ξ(^{31}P) = 40.480742 (H_3PO_4).

Pulse programs
All pulse programs used are standard Bruker NMR pulseprograms except for the R_1 measurements.

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/noesygpphpp; 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, $^{1}J_{XH}$ = 145 Hz; TD = 4096; increments = 512 - 1k;

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

2D-^{1}H,^{31}P HMBC: Pulse program: inv4gplrndqf; Relaxation delay = 4 - 8 s, NS = 8-32, TD = 4096; increments = 256 - 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;

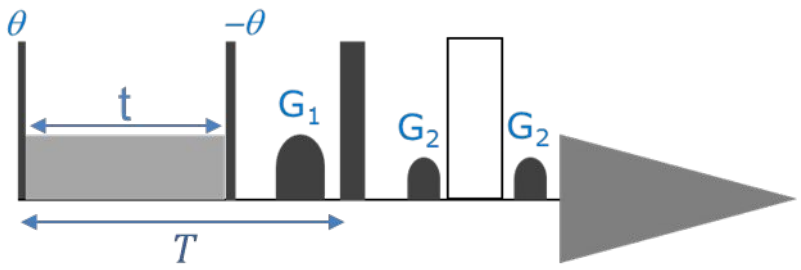
^{19}F-NMR: Pulse program: zg30; Relaxation delay = 2 – 3 s, Acquisition time = 11.60 s, SW = 10.0 ppm, TD = 128k, NS = 8 – 64;

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;

1D ^{1}H off-resonance $R_{1\rho}$

Pulse Sequence

The recent reported 1D ^{1}H off-resonance $R_{1\rho}$ pulse sequence is adopted with slight modification for our measurement.[6,7]



$$R_{1\rho} = -\frac{1}{T} ln \frac{I}{I_0}$$

Figure 1: Applied pulse sequence and mathematical relation to measure $R_{1\rho}$ experimenally. The applied angle (θ) is 35°. A spinlock period (t) of 100 ms is applied. The filled (black) and unfilled rectanglur pulses respectively indicate 90° and 180° hard pulses. The gradient pulses of G_1 = 70 % and G_2 = 40 % of the maximum were applied. I_0 is the intensity without any spinlock period and I is the intensity with spinlock period measured over a multiple effective magnetic filed.

Parameter Optimization

The spinlock period (t) was incremented in 10 ms steps with maximum spinlock power (≈ 20 kHz). At each step, the temperature was monitored (sample heating can occur due to application of high intensity spinlock field over an extended time). Around 120 ms, temperature oscillation was observed. To avoid any influence of temperature changes on the measurement, the spinlock period of 100 ms was applied in all our measurements.

The normal relaxation period (T-t) in the absene of the spinlock is tested for 3 delays (50 ms, 100 ms and 150 ms). For all three different relaxation periods (T-t), we found similar exchange rates within the experimantal errors. To minimise signal loss due to relaxation, (T-t) of 50 ms was used in all our measurements.

Method testing

To test the applicability of the $R_{1\rho}$ method, we applied the above described pulse sequence with optimized parameters on the known peak in the spectrum (*para*-methyl protons of the hydrolyzed imine ketone part), which does not experience any chemical exchange process (on a ms-µs timescale) and on the same proton for the CPA/imine complex which experiences chemical exchange. The measured rate for the hydrozyled ketone showed a nearly straight line (no offset-Lorentzian decay with increasing effective field ω_{eff}), which was expected for non exchanging protons. For the same proton in the binary CPA/imine complex, an offset-Lorentzian decay was observed, which demonstrates the presenence of chemical exchange on a ms-µs timescale.

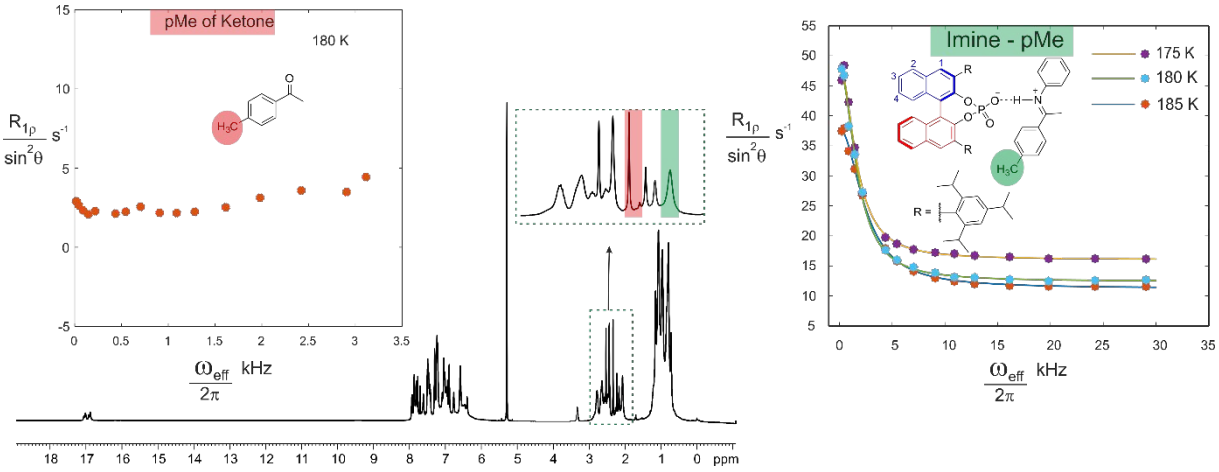


Figure 2: To test the method, we selected the proton peak of the *p*-methyl group in the hydrolyzed ketone moiety (red shaded) and the proton peak of the *p*-methyl imine in the TRIP/imine binary complex (green shaded) within the same sample (to maintain identical conditions). The hydrolyzed ketone does not undergo any chemical exchange on a ms-µs time scale. The corresponding measured $R_{1\rho}$ data at 180 K with incremental effective field showed a near horizontol line, proving the absence of chemical exchange (left side). On the other hand, the imine inside the catalyst undergoes $E_I \rightleftharpoons E_{II}$ exchange and thus the corresponding $R_{1\rho}$ data at 185, 180 and 175 K with incremental effective field showed offset-Lorentzian decays for the *p*-methyl protons in the TRIP/imine complex. This confirms the presence of chemical exchange process and hence validates our method for chemical exchange detection in ms-µs range.

Curve fitting

In order to analyze the $R_{1\rho}$ measurements, the signal intensities (integrals) are determined for every effective field strength ω_{eff} (i.e. every different spinlock power) and normalized to the reference intregral (spinlock power = 0 W). Initially, to extract k_{ex}, the measured experimental points are curve fitted to the following theoretically described equation by using MATLAB (see literature for further details[8]).

$$\frac{R_{eff}}{\sin^2\theta} = R_2 - R_1 + \frac{(\Delta\omega)^2 P_A P_B \tau_{ex}}{\left(1 + \tau_{ex}^2 \omega_{eff}^2\right)} \qquad (Eq.\ 1)$$

Here R_2 *is the tranverse relaxation rate constant*

R_1 *is the longitudinal relaxation rate constant*

$\Phi = (\Delta\omega)^2 P_A P_B \tau_{ex}$ *encodes both chemical shift differnce and population of the minor* (P_B) *and major* (P_A) *exchange species*

Φ and the average isotropic chemical shift Ω (in ppm) are related by

$$\Phi = -\Omega^2 + a\Omega + b \qquad (Eq.\ 2)$$

Here,

$a = 2\Omega_A - \Delta\omega$

$b = \Omega_A(\Delta\omega - \Omega_A).$

These can be rearranged as

$$\Delta\omega = (a^2 + 4b)^{1/2}, \text{ and } \Omega_{A,B} = [a \pm ; (a^2 + 4b)^{1/2}]/2 \qquad (Eq.\ 3)$$

Φ and Ω can be obtained experimentally at different temperatures. Assuming the chemicalshift difference $\Delta\omega$ between major (A) and minor (B) species is constant, one can calculate $\Delta\omega$. From $\Delta\omega$ value and Φ values, populations can be extractable.

Directionality

For the chemical exchange between A and B, the exchange rate constant k is: $k_{ex} = k_A + k_B$. By using populations and k_{ex} one can extract rate constants k_A and k_B on both sides.

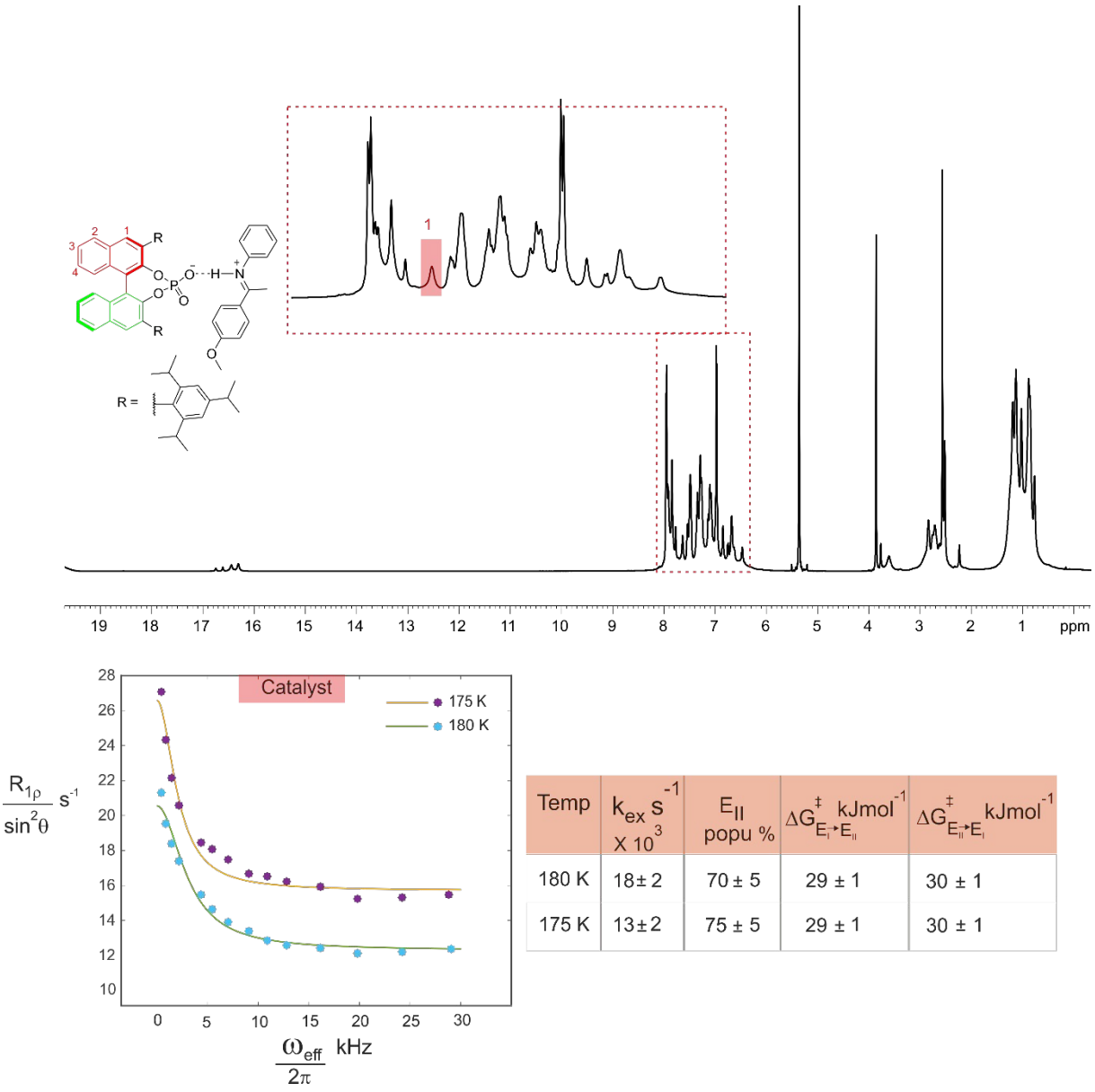
$$A \underset{k_B}{\overset{k_A}{\rightleftharpoons}} B \qquad P_A = \frac{k_B}{k_A + k_B} \qquad P_B = \frac{k_A}{k_A + k_B}$$

If a temperature independence within the varied range of 10 K is assumed, then the coefficients *a* and *b* can be determined by least squares optimization. Subsequently, $\Delta\omega$ is calculated by $\Delta\omega = (a^2 + 4b)^{1/2}$, and $\Omega_{A,B} = [a \pm ; (a^2 + 4b)^{1/2}]/2$. Once $\Delta\omega$ is known, P_A, P_B, k_A and k_B are obtained from Φ_{ex} and k_{ex} at each temperature.

Hence, in order to seperate the populations and chemical shift difference from the term ϕ, it requires additional experimental $R_{1\rho}$ measurements at more than one temperature. Therefore we measured $R_{1\rho}$ experiments for each sample at two or three temperatures (185 K, 180 K and 175 K).

Results of the $R_{1\rho}$ measurements

TRIP/3

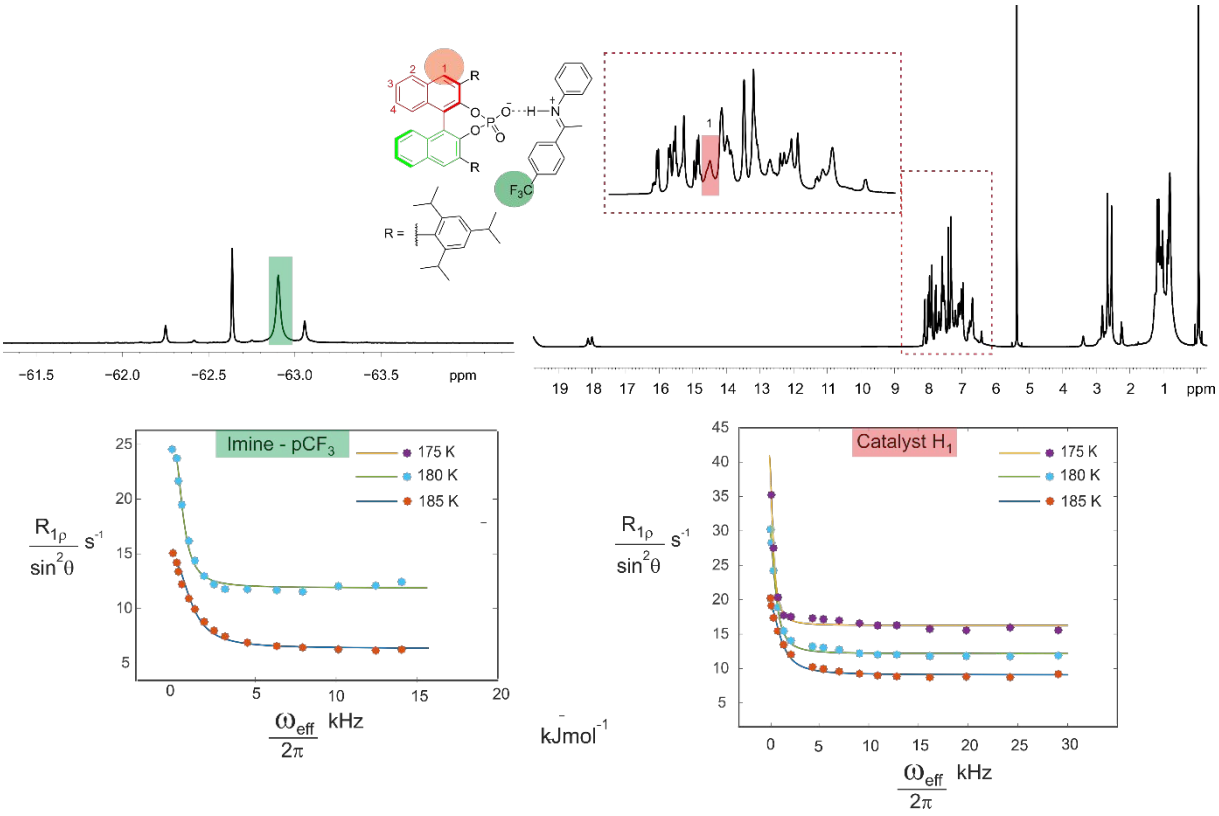


Temp	k_{ex} s^{-1} X 10^3	E_{II} popu %	$\Delta G^{\ddagger}_{E_I \to E_{II}}$ kJmol^{-1}	$\Delta G^{\ddagger}_{E_{II} \to E_I}$ kJmol^{-1}
180 K	18± 2	70 ± 5	29 ± 1	30 ± 1
175 K	13± 2	75 ± 5	29 ± 1	30 ± 1

Figure 3: $R_{1\rho}$ measurement for the TRIP/**3** complex. The proton H_1 of the catalyst (marked in the spectrum, red shaded) was selected as probe. The offset-Lorentzian decay indicates the

pesence of chemical exchange (k_{ex} ≈18000 s^{-1} at 180 K). With experimental data obtained at two different temperatures, the populations and directionality were extracted.

*TRIP/**2***



kJmol^{-1}

Temp	k_{ex} s^{-1} X 10^3	E_{II} popu %	$\Delta G^{\ddagger}_{E_I \to E_{II}}$ kJmol^{-1}	$\Delta G^{\ddagger}_{E_{II} \to E_I}$ kJmol^{-1}
185 K	6 ± 1	76 ± 5	30 ± 1	32 ± 1
180 K	3.5± 1	88 ± 5	30 ± 1	32 ± 1

Temp	k_{ex} s^{-1} X 10^3	E_{II} popu %	$\Delta G^{\ddagger}_{E_I \to E_{II}}$ kJ	$\Delta G^{\ddagger}_{E_{II} \to E_I}$ kJmol^{-1}
185 K	9± 1	74 ± 5	31 ± 1	33 ± 1
180 K	5 ± 1	78 ± 5	31 ± 1	33 ± 1
175 K	2.5±1	83 ± 5	31 ± 1	33 ± 1

Figure 4: $R_{1\rho}$ measurement for TRIP/**2** complex. The proton H_1 of the catalyst (shaded in red) and the fluorine signals of the imine-CF_3 group (shaded in green) were selected as probes. The offset-Lorentzian decay indicates pesence of chemical exchange (k_{ex} ≈ 3-5·10^3 s^{-1} at 180 K). With experimental data obtained at three different temperatures, the populations and directionality were extracted.

*TiPSY/**1***

Temp K	k_{ex} s^{-1} x 10^{-3}	E_{II} %	$\Delta G^{\ddagger}_{E_I \rightarrow E_{II}}$ kJ mol^{-1}	$\Delta G^{\ddagger}_{E_{II} \rightarrow E_I}$ kJ mol^{-1}
185	3.0 ± 1	95 ± 5	32 ± 1	36 ± 1
180	2.5 ± 1	96 ± 4	32 ± 1	36 ± 1
175	2.5 ± 2	95 ± 5	31 ± 1	35 ± 1

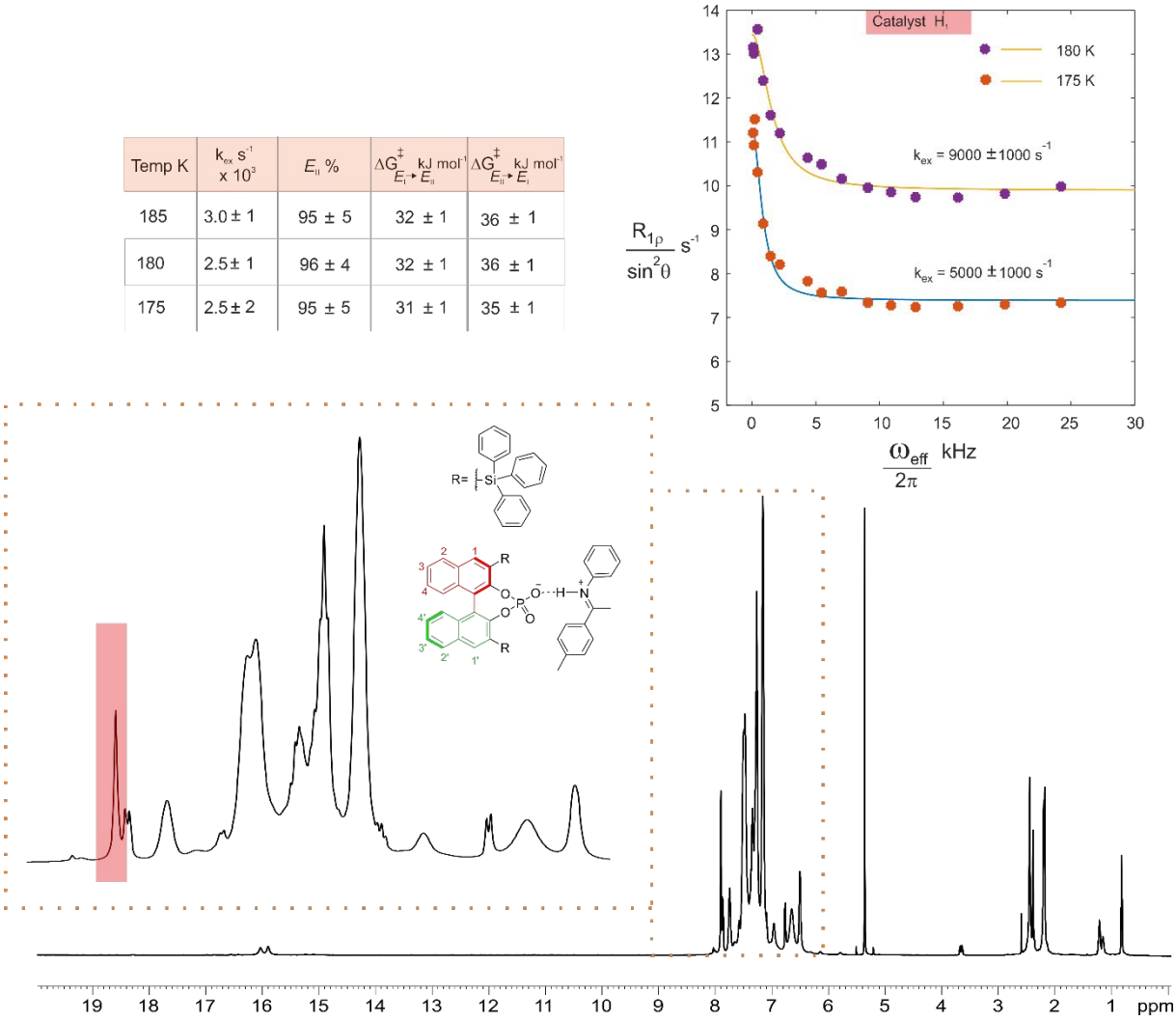


Figure 5: $R_{1\rho}$ measurement for TiPSY/**1** complex, (to avoid signal overlap, the sample was prepared with nearly exclusive population of the *E*-complex; see above for sample preparation). The proton H_1 of the catalyst (shaded in red) was selected as probe. The offset-Lorentzian decay indicates pesence of chemical exchange ($k_{ex} \approx 9$ ks^{-1} at 180 K).

*TRIM/**2** and TRIM/**3***

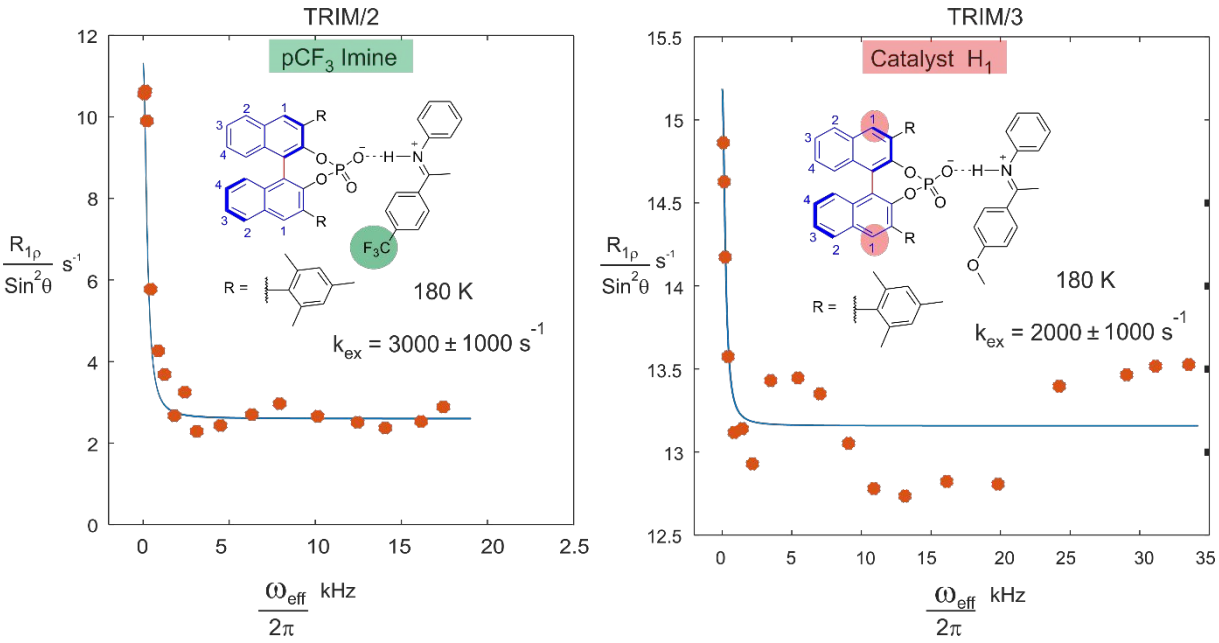


Figure 6: $R_{1\rho}$ measurements for TRIM/**2** and TRIM/**3** complexes. For TRIM/**2**, the CF_3 group of the imine was used as a probe (shaded in green) and for TRIM/**3** the proton H_1 of the catalyst (shaded in red) was selected as probe. The offset-Lorentzian decay in both system indicates the pesence of chemical exchange ($k_{ex} \approx$ 2000-3000 s^{-1} at 180 K).

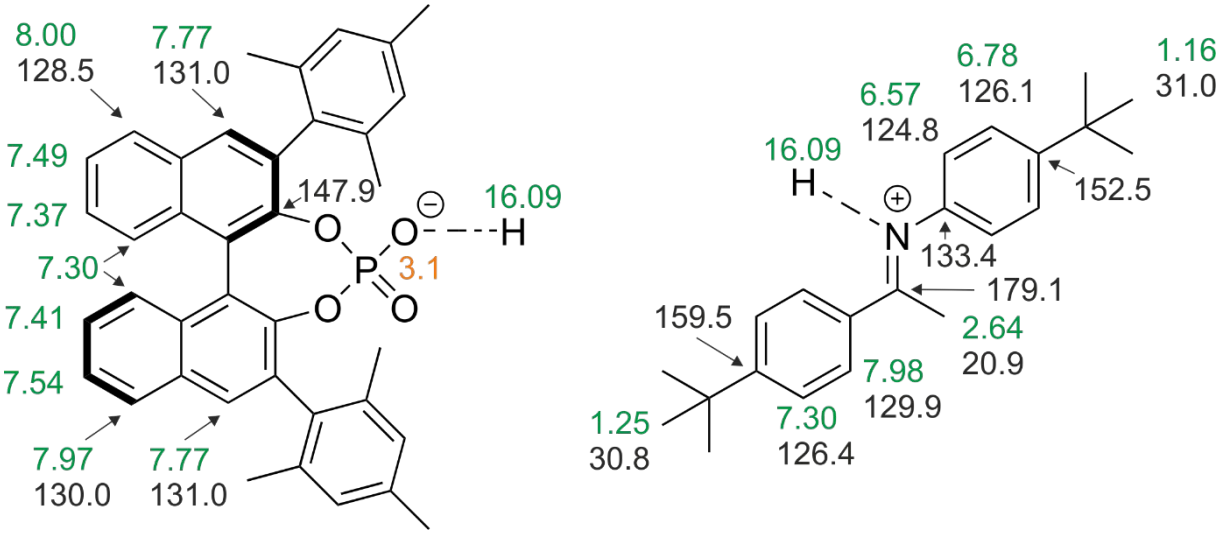
For TRIM/**2** and TRIM/**3**, the offset-Lorentzian decay fit does not match the experimental decay as precisely as for the other systems. Hence, a larger experimental error is expected. However, the $R_{1\rho}$ measurements for TRIM/**2** and TRIM/**3** complexes indicate, that similar exchange rates ($k_{ex} \approx$ 2000-3000 s^{-1} at 180 K) are obtained for TRIM/**1**-**3** regardless of the hydrogen bond strength.

NMR-Structural analysis of CPA/imine complexes

The investigated complexes TRIP/**1**-**3**, TiPSY/**1** and TRIM/**1**-**3** were already described in the previous work.[2,9] The NMR-structural analysis of TRIM/**4** is described below. In addition, the backbone splitting of TiPSY/**1** is discussed in detail below.

*Chemical Shift assignment of TRIM/**4***

The ^{1}H (black) and ^{13}C (green) chemical shifts (in ppm) 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. The ^{31}P (orange) chemical shift (in ppm) was assigned by ^{1}H,^{31}P HMBC. Due to signal overlap and lacking resolution and intensity of 2D correlations, not all signals could be assigned.



In accordance with our previous analysis of hydrogen bond strengths,[1] the ^{1}H chemical shift of the hydrogen bond strength reflects the H-bond strength (in our system, higher chemical shifts correlate with stronger H-bonds). Hence, the H-bond strength of TRIM/**4***E* (16.09 ppm) is in between TRIM/**1***E* (16.26 ppm) and TRIM/**3***E* (15.80 ppm).[9]

Identification of Type I E and Type II E

Analogous to our previous work,[2,9] for the *Type I E* structure, the *tert*-butyl group of the ketone part of the imine (marked in blue) is placed above the BINOL backbone. The blue NOE cross signals A and B to the Naphthyl backbone reveal the presence of the *Type I E* structure (Figure 7) for TRIM/**4***E*. The NOE cross signal D (black) is a result of overlapping NOE signals between the *tert*-butyl group and the naphthyl backbone and the *tert*-butyl group and the attached

phenyl ring (backbone: 8.00 ppm, phenyl ring of imine: 7.98 ppm). For the *Type II E* structure, the tert-butyl group of the aniline part of the imine is placed above the BINOL backbone and thus the red NOE cross signals A-D reveal the presence of the *Type II E* structure.

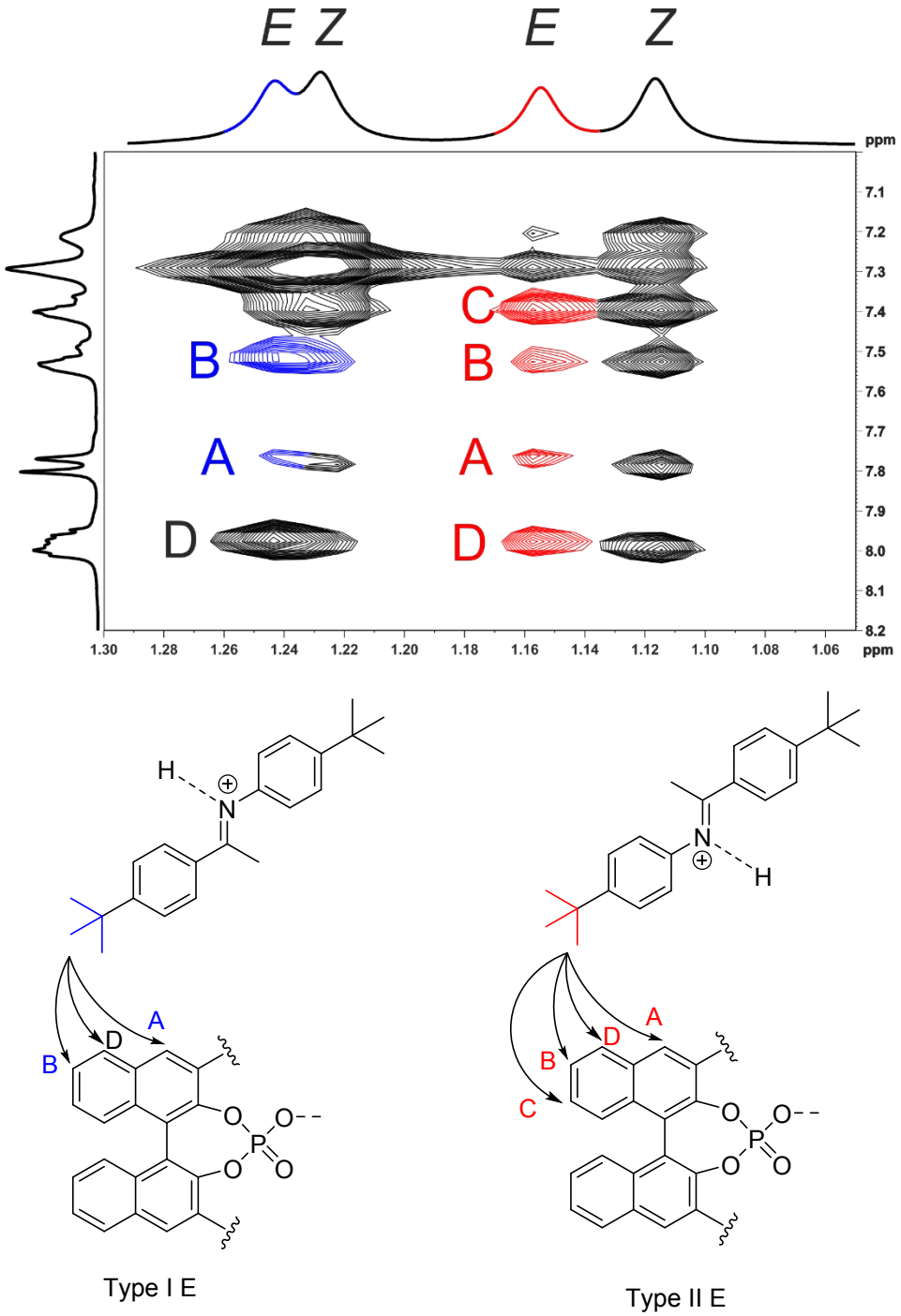


Figure 7: Excerpt of the $^{1}H,^{1}H$ NOESY spectrum of TRIM/**4** at 180 K and 600 MHz (100 mM sample) in CD_2Cl_2. The blue NOE cross signals indicate the presence of the *Type I E* structure, while the red NOE signals indicate the presence of the *Type II E* structure.

*DOSY measurements of TRIM/**4***

To prove, that the observed species in TRIM/**4** are monomers of the binary complexes, DOSY measurements (Difusion ordered spectroscopy) were performed to derive the molecular radii of the present species.

The DOSY measurements were performed with the convection suppressing DSTE (double stimulated echo) pulse sequence developed by Jerschow and Müller in a pseudo 2D mode.[10] TMS was used to reference the viscosity of the solvent at 180 K. The diffusion time delay was set to 45 ms. The gradient pulse lengths (p16, SMSQ10.100 pulse shape) were optimized for each species to give a sigmoidal signal decay for varying gradient strengths. Optimal pulse lengths of 3.0 ms and 6.0 ms were found for TMS and TRIM/**4**, respectively. For each species, twenty spectra with linear varying gradient strength of 5% - 95% have been measured. The used probe signals for the analysis are listed in table 1. The signal intensities of the respective groups were analyzed as a function of the gradient strength by Bruker TopSpin 3.2 software T1/T2 relaxation package by employing the Stejskal-Tanner equation.[11] No line broadening occurred for increasing gradient strength. The sigmoidal fit provided the translational self-diffusion coefficients D_i listed in Table 1. The molecular radii were derived by the Stokes-Einstein equation[12] using Chens correction.[13]

$$D_i = \frac{k_B T}{6\pi\eta r_H} * (1 + 0.695 * (\frac{r_{solv}}{r_H})^{2.234} \qquad (Eq. 4)$$

D_i is the self-diffusion coefficient derived by the measurement, η is the viscosity of the solvent, r_H is the hydrodynamic radius of the observed molecule and r_{solv} the radius of the solvent . No form factor correction was applied. The viscosity was determined by measuring the diffusion coefficient of the reference tetramethylsilane (TMS) and solving the equation for η with the literature value[14] of the radius of 2.96 Å. The solvent radius of CD_2Cl_2 (2.46 Å) was taken from the reference.[15]

Table 1: Probe signals, measured diffusion coefficients and derived molecular radii for TRIM/**5**.

Entry	Species	p16 [ms]	Observed signal [ppm]	D_i [m^2/s] $\cdot 10^{-12}$	Averaged	r_H [Å]
1	TMS	3.10	0.00	21.32		
2	TRIM/**4***E*	6.00	1.16	4.76		
3	TRIM/**4***E*	6.00	2.64	4.80	4.69	9.54
4	TRIM/**4***E*	6.00	7.77	4.50		

The derived molecular radius (9.54 Å) is similar to the one reported previously for TRIM monomers.[9] Thus, the DOSY measurements showed, that the species investigated by the $R_{1\rho}$ measurement is the binary TRIM/**4***E* complex.

Estimation of the rotational correlation time of binary CPA/imine complexes

A general rotational correlation time of 10-50 ns was estimated for the investigated binary complexes of chiral phosphoric acids and imines with their hydration shell. Stokes Law (Eq. 5) was used to calculate the rotational correlation time based on the results of the DOSY measurements of TRIM/**4***E*.

$$\tau_c = \frac{4\pi\eta r^3}{3kT} \qquad (Eq.\ 5)$$

The radius of the binary complex of TRIM/**4** with its hydration shell was determined by DOSY measurements (see respective chapter) and a radius of 9.54 Å was determined for the complex with its hydration shell. The viscosity ($3.05*10^{-2}$ kg m^{-1} s^{-1}) of the solution at 180 K was determined by Equation 4 based on the DOSY measurement on TMS. A rotational correlation time of 44.6 ns was calculated for TRIM/**4***E* with its hydration shell. Given the bulkiness of the two tert-butyl substituents of imine **4**, it is expected that the other investigated complexes have smaller radii, resulting in smaller rotational correlation times. Hence, a general rotational correlation time around 10 – 50 ns was estimated.

*TiPSY/**1***

In the TiPSY/**1** complex, the backbone splitting could not be resolved at 180 K and 600 MHz in CD_2Cl_2 (see figure). However, in our previous investigations we observed, that the backbone splitting in TiPSY complexes is very small and could often not be resolved sufficiently (see SI of literature).[9] Goodman *et al.* demonstrated, that the binding pocket for TiPSY is significantly smaller than for TRIP (no rotation possible).[16] The biggest binding pocket for the investigated CPAs was determined for TRIM (rotation possible). Hence, a rotation of the imine inside the binding pocket of TiPSY can be excluded, even if the backbone splitting can not be resolved sufficiently.

The sample was prepared with an exclusive population of the *E*-imine. To achieve that, the sample was prepared according to the general procedure described above. However, before adding the solvent, the NMR-tube with TiPSY and **1** was cooled to -90 °C in acetone/liquid N_2 and the precooled solvend was added to the tube. The low temperature suppressed *E*→*Z* isomerization of the imine.

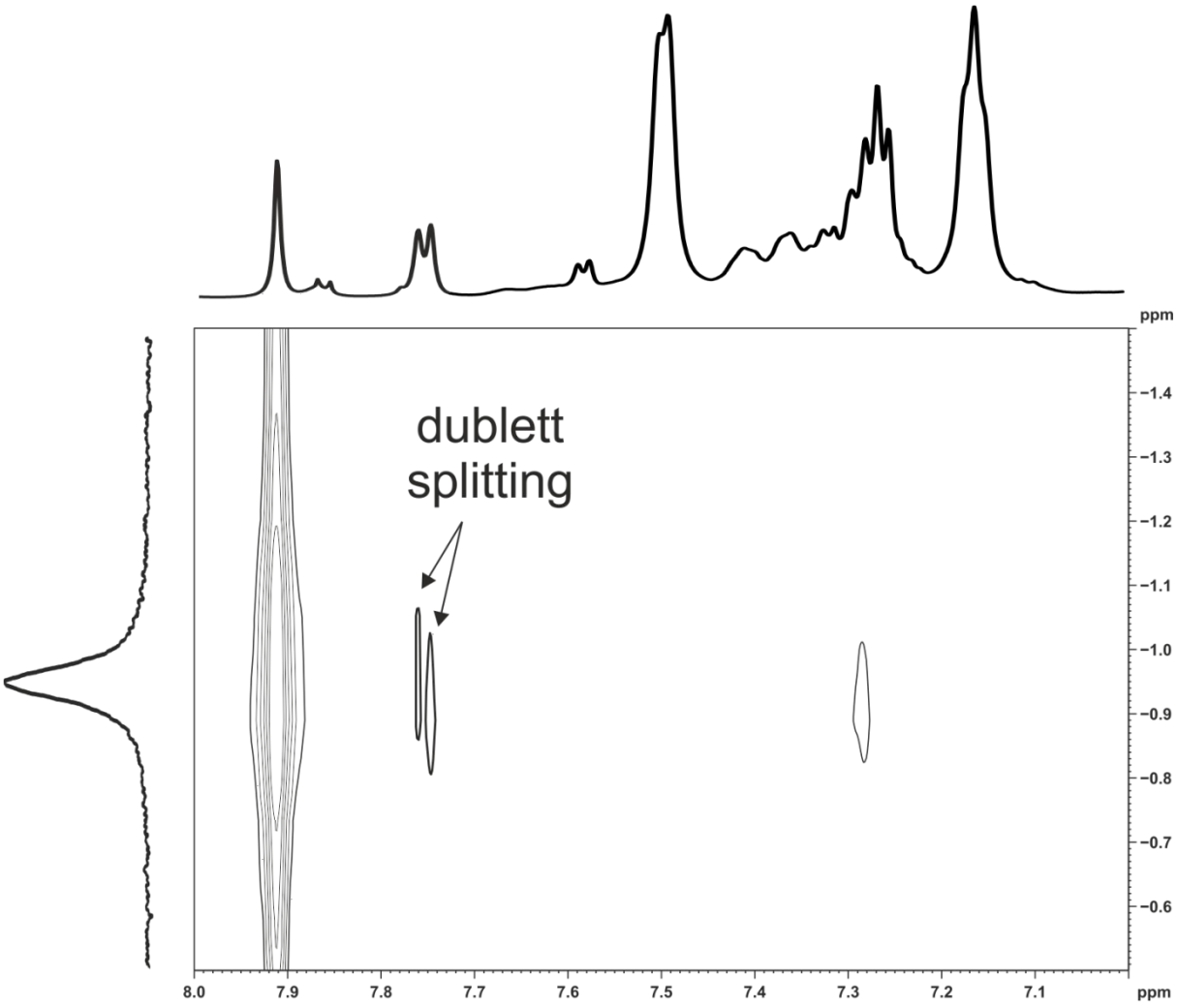


Figure 8: Excerpt of the $^{1}H,^{31}P$ HMBC spectrum of TiPSY/1 (E-only, 25 mM, TiPSY:**1** = 1:1) at 180 K and 600 MHz in CD_2Cl_2. The sample was prepared with an exclusive population of *E*-imine species.

Exchange with free imines

Typically, in 1:1 complexes of TRIP, TRIM and TiPSY, the complexation of the imine was incomplete (≈ 25 % free imine present). Thus, for complexes with imines **1**-**3**, the assignment of the free imines was done for the CPA/imine samples. For imine **4**, a NMR sample with the imine only (50 mM, CD_2Cl_2, 180 K and 600 MHz) was measured and compared to the chemical shifts in the CPA/**4** sample. For TRIM/**4**, no free imine was observed in the binary complex sample.

As the free imines **1**-**4** gave chemical shifts well separated from the respective CPA/*E*-imine complexes (see figure 9 for free imines and assignments of the binary complex in literature[2,9]), the exchange between free and complexated imine is slow on the NMR time scale. Thus, the exchange pathway via dissociation and re-association causing averaging of the BINOL backbone can be excluded to significantly contribute to the measured exchange rates in the $R_{1\sigma}$ measurements.

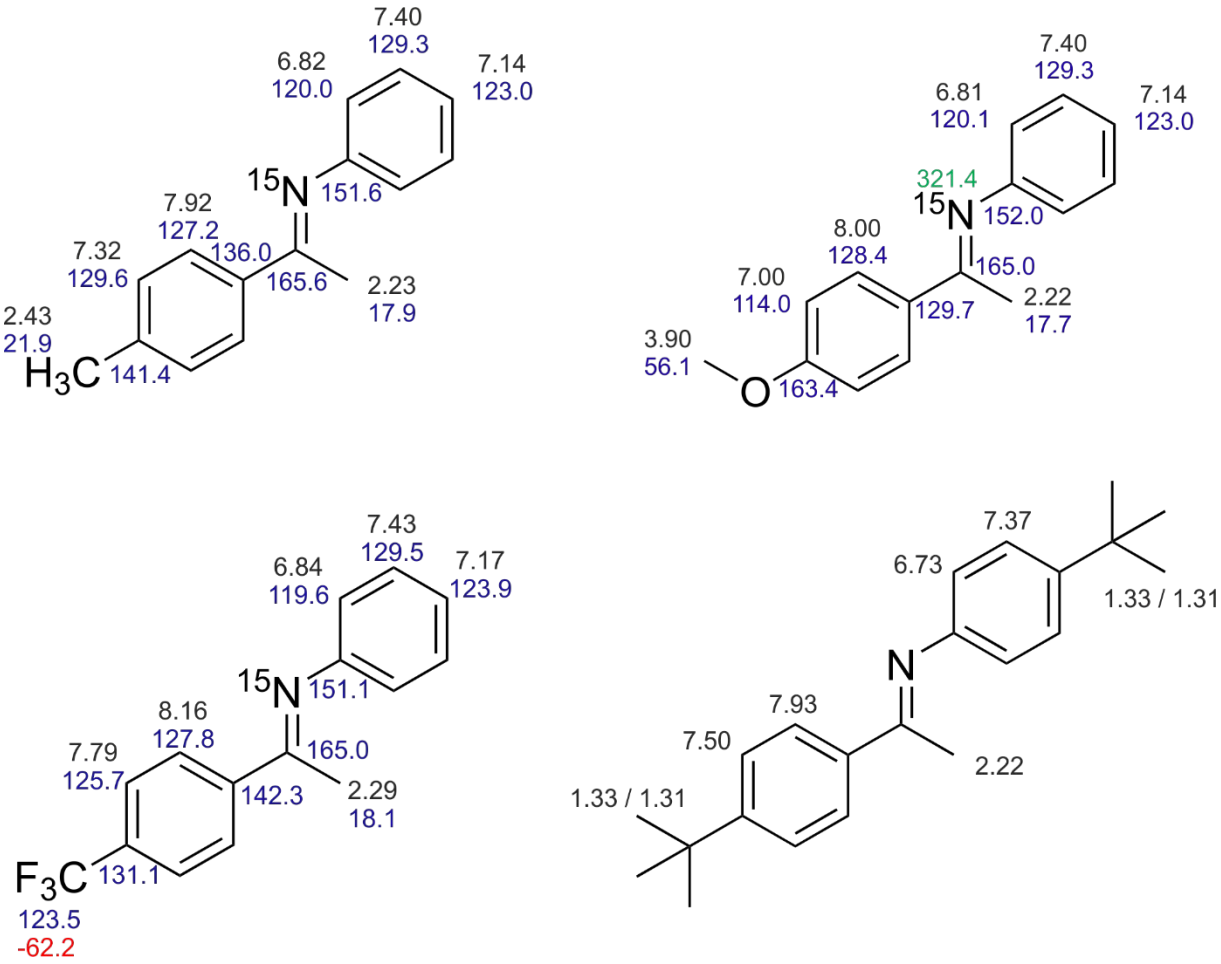


Figure **9**: Chemical shift assignment of the free imines **1**-**4** at 180 K in CD_2Cl_2.

Additional fitting of TRIM/**1***E*

Due to the strong signal decay within the first few percent of the horizontal axis for TRIM/**1***E* (Figure 6B in the manuscript), fewer data points are in the decay region relevant for the fit, which could affect the quality of the fit and thus the precision of the extracted rate. However, the fit curves for lower (500 s^{-1}) and higher (10 000 s^{-1}) exchange rates as the optimized one (2500 s^{-1}) significantly deviate from the data set (Figure 10).

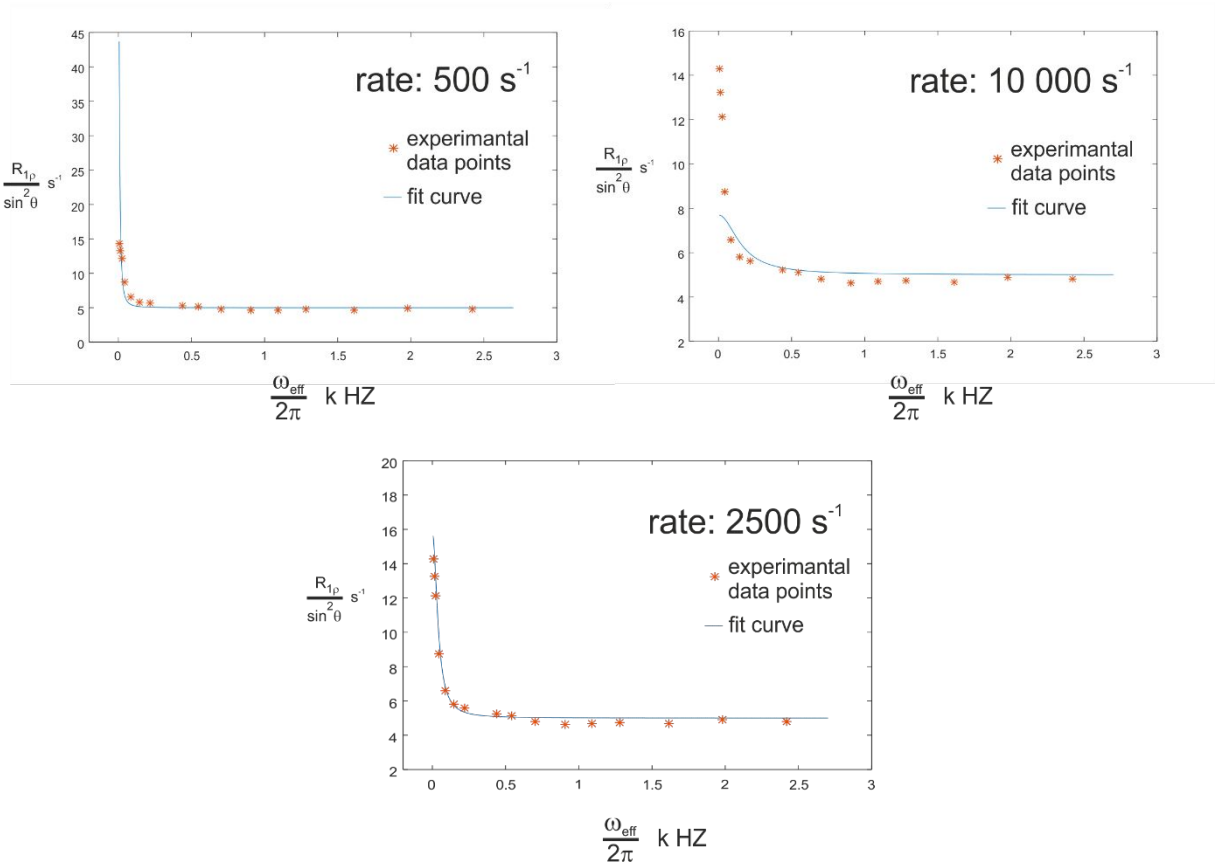


Figure **10**: Additional curve fitting for the signal decay of TRIM/**1***E* with different exchange rates at a concentration of 5 mM. The determined exchange rate of 2500 s^{-1} fits the data set best, while lower or higher exchange rates result in a significant offset. Other parameters, e.g. the population of *E*-I and *E*-II were not changed.

In addition, a TRIM/**1***E* sample at different concentration (0.25 mM) was measured with more ω_{eff} increments. The exctracted exchange rate of 2500 s^{-1} is identical to the previous one and the fit for lower or higher exchange rates does not match the data set (Figure 11).

Hence, the quality of the fit for TRIM/**1***E* is adequately precise to reveal, that the exchange rate for TRIM/**1***E* is significantly lower than for TRIP/**1***E* (≈10 000 s^{-1}).

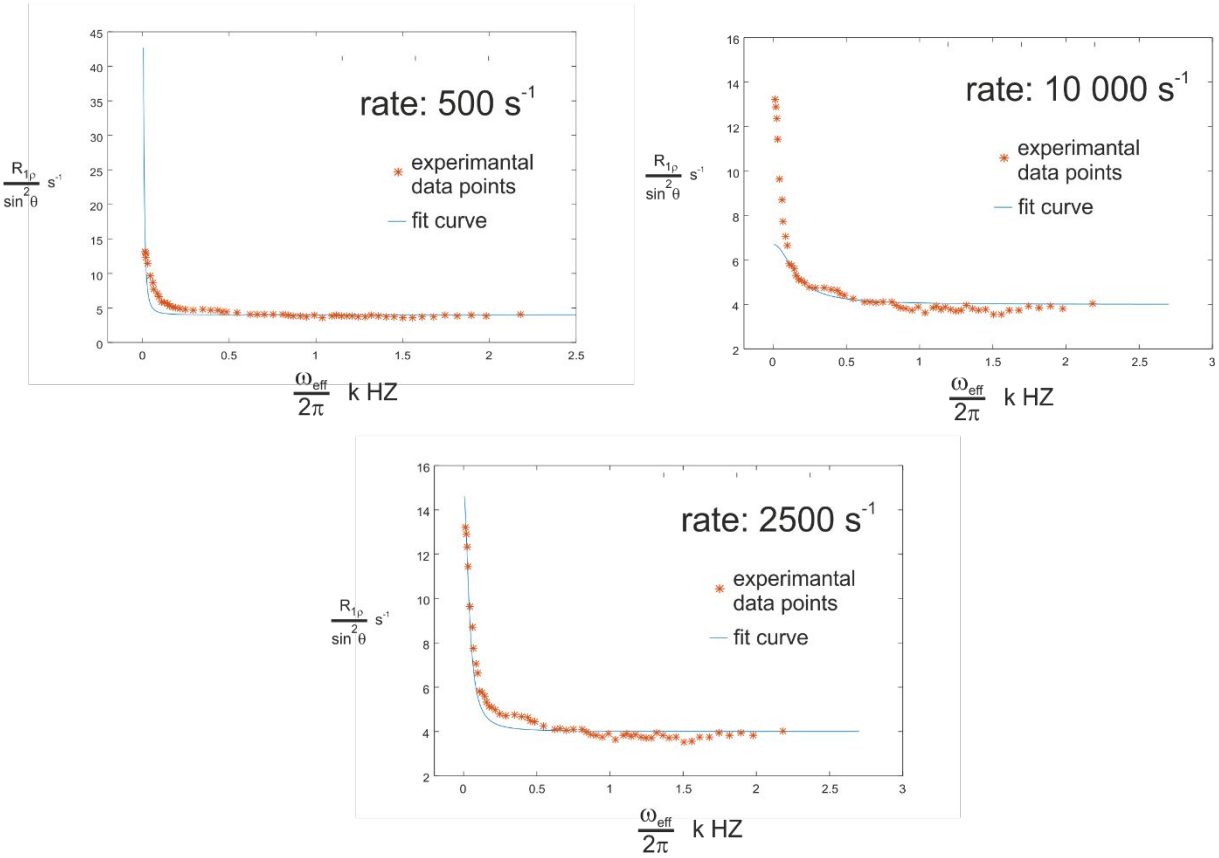


Figure **10**: Additional curve fitting for the signal decay of TRIM/**1***E* with different exchange rates at a concentration of 0.25 mM and additional ω_{eff} increments. The determined exchange rate of 2500 s^{-1} fits the data set best, while lower or higher exchange rates result in a significant offset. Other parameters, e.g. the population of *E*-I and *E*-II were not changed.

Computational Details

All structures were optimized at TPSS/def2-SVP[17] level of theory using D3[18] correction in continuum of CH2Cl2 (SMD[19]). The dielectric constant was adapted to 16.20 to mimic low temperature condition in the experiment. Vibrational and thermochemical analyses were performed at the same level of theory as the geometry optimization. Subsequently, single point calculations at SCS-MP2/CBS[20] level of theory were conducted. Def2-SVP and def2-TZVP basis sets were used for extrapolation to approach complete basis set. Solvent and thermochemical corrections were added to the single point energy. Software used for the geometry optimization, frequency analysis and solvent correction was Gaussian 09 version D.01.[21] For single point calculation, ORCA 4.1.1 was used.[22] Constant temperature (NVT) molecular dynamic was done using semi-empirical xtb software in DCM.[23]

Extrapolation procedure

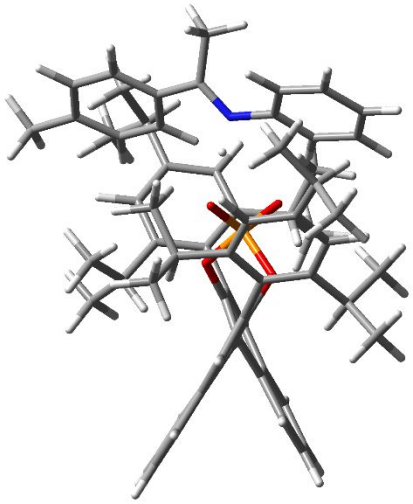
The CBS basis set extrapolation proceeds under the two point extrapolation procedure as in implemented in ORCA 4.1.1 with the basis set Def2-SVP and Def2-TZVP.

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

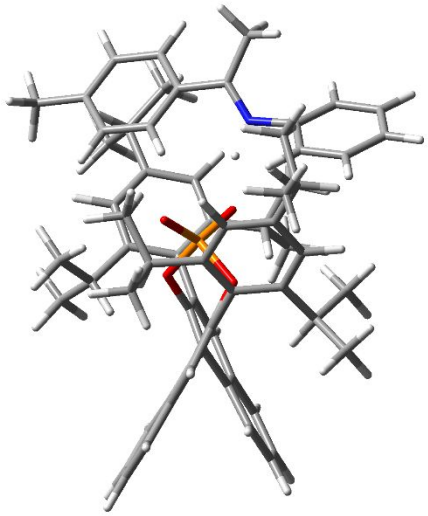
$$E_{\mathrm{corr,MP2}}^{\infty} = \frac{X^{\beta}E_{\mathrm{corr,MP2}}^{X} - (X-1)^{\beta}E_{\mathrm{corr,MP2}}^{X-1}}{X^{\beta} - (X-1)^{\beta}}$$

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

TRIP/1E Type III.1 and E-III.2 structures (most stable conformations)



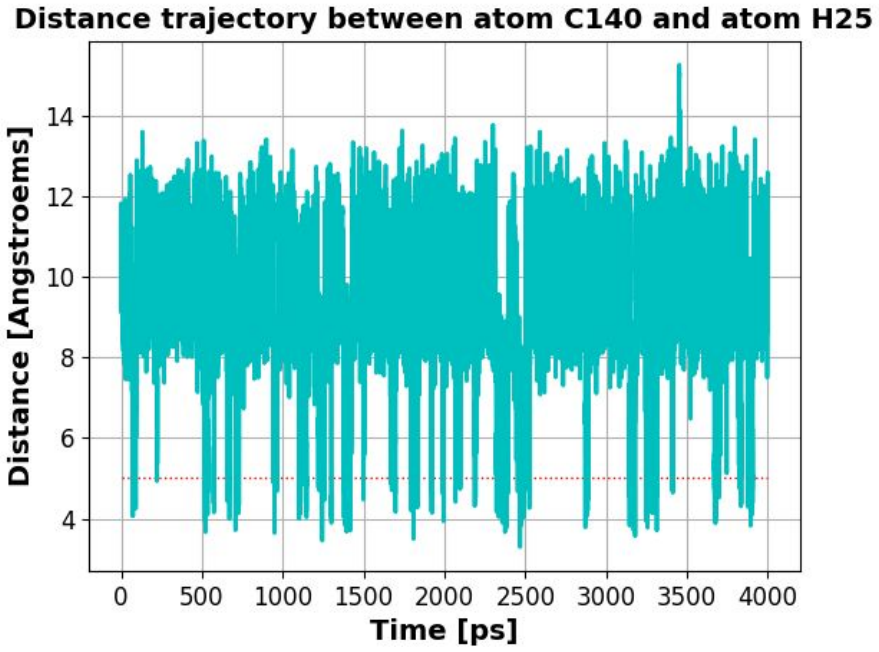
Type E-III.1

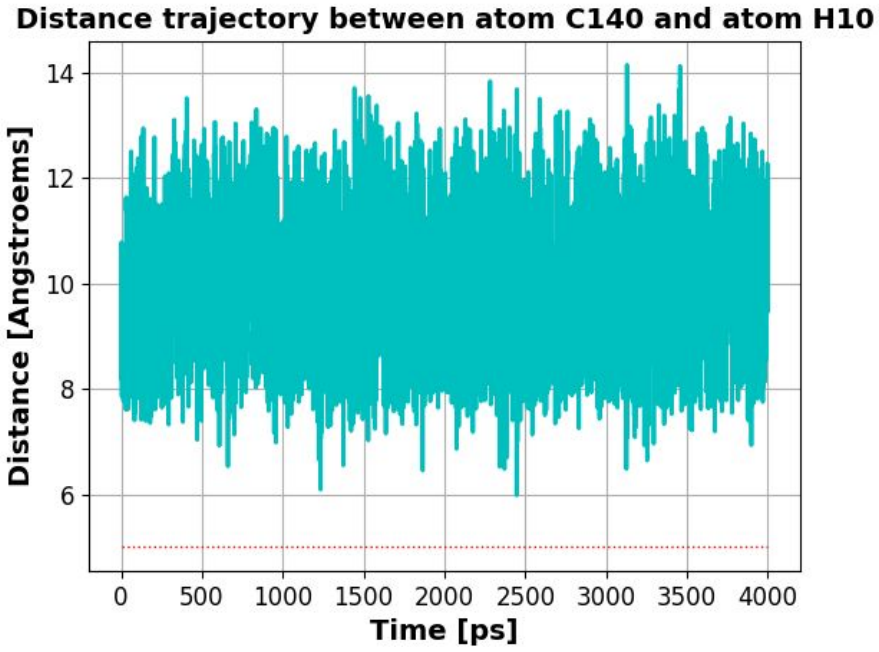


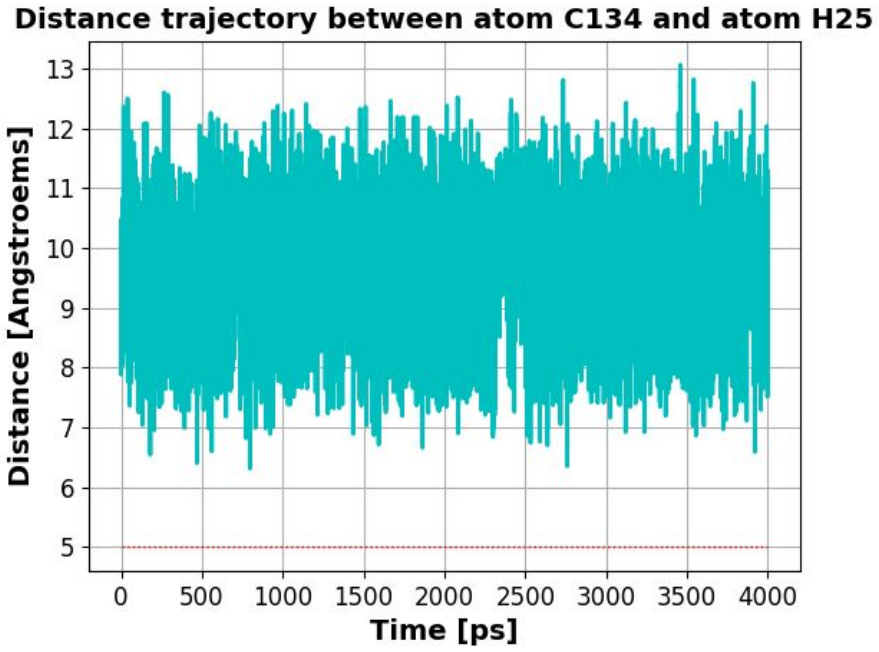
Type E-III.2

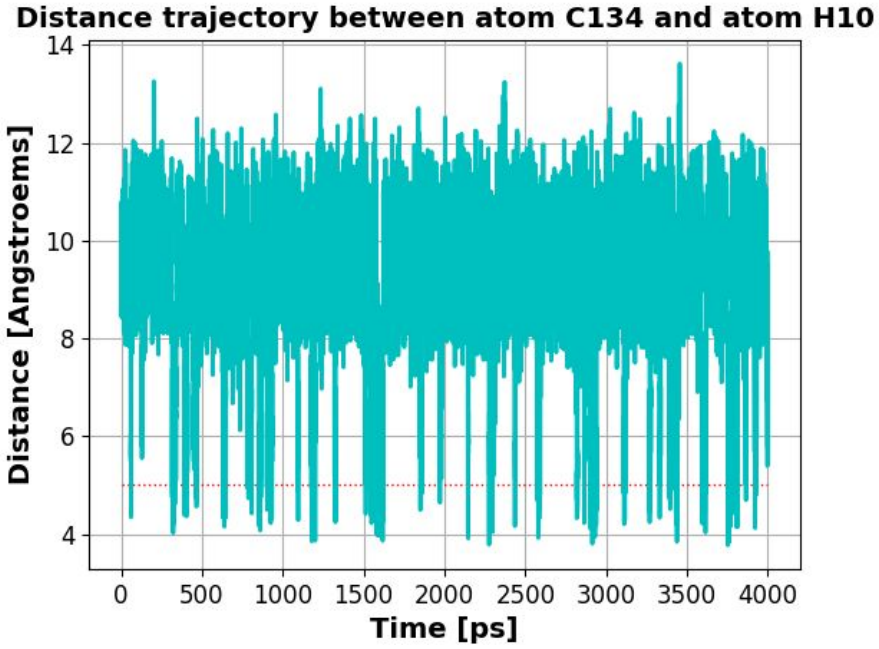
xtb-MD of TRIP/1E binary complex at 370 K

MD of TRIP/1E complex shows the exchange of E-II and E-I conformations via tilting and switching. The E-II conformation is marked by the close contact between C134 and H10, while the E-I conformation shows close contact between C140 and H25. No rotation is observed during a simulation of 4000 ps at 300 K to 370 K, i.e. C134 never meets H25 or C140 never meets H10. Beyond this temperature, dissociation of complex is observed.









Optimized Geometries

TRIM/1E Type I

1\1\GINC-WORKER0\FOpt\RTPSSTPSS\def2SVP\C53H48N1O4P1\JHIOE\24-Apr-2018
\0\\#p tpsstpss/def2svp empiricaldispersion=gd3 int=ultrafine opt scrf
=(smd,solvent=ch2cl2,read)\\title\\0,1\P,-0.1297143417,-0.4860433703,-
1.1839383304\O,-1.4175075558,0.5618941922,-1.4320413577\O,0.6889832102
,0.3763631976,0.0168282895\O,0.6300817555,-0.5399021282,-2.4784978792\
O,-0.5766080585,-1.7420153175,-0.4359277394\C,-1.446100498,2.147809437
,0.3711360845\C,-2.0698317941,1.122837238,-0.3502138217\C,-3.395018365
8,0.6663965667,-0.0681477603\C,-4.0703770977,1.2454430496,0.9985929916
\H,-5.095082782,0.9299435094,1.2232029452\C,-3.4593497944,2.2287931273
,1.8282185621\C,-2.1205478813,2.6764874421,1.5309470667\C,-1.502671696
6,3.5956395341,2.4329780968\H,-0.4706962922,3.9085577634,2.251357641\C

,-2.1840971756,4.0819139807,3.5389827427\H,-1.6850717191,4.7804794202,
4.2194778391\C,-3.5190578898,3.6730083748,3.8040883989\H,-4.0466914589
,4.0672317544,4.679316788\C,-4.1381357835,2.7585716694,2.9673759161\H,
-5.1579812303,2.4147168377,3.1741719223\C,-0.0995474827,2.6345132883,-
0.0476174044\C,0.9455071297,1.7164195775,-0.1873343455\C,2.2926672419,
2.1001225065,-0.4723187204\C,2.558703778,3.4483819763,-0.6657499207\H,
3.5849117489,3.7741013745,-0.8683863455\C,1.5225638135,4.4269654309,-0
.627942795\C,0.1688315104,4.0227443182,-0.3306877178\C,-0.8544115593,5
.0185025682,-0.3633523236\H,-1.891720726,4.7236493662,-0.1814759087\C,
-0.5547814947,6.3456273979,-0.6331615051\H,-1.3588983494,7.0894174279,
-0.6571408924\C,0.7839495245,6.7474855465,-0.8872017123\H,1.0082027204
,7.7998634367,-1.092917887\C,1.798284324,5.8032516275,-0.889462277\H,2
.8323097674,6.0967771622,-1.1038106254\C,-0.8573168791,-0.0871264197,4
.830477067\C,0.3250076425,-0.6640802772,5.339846067\H,0.5983745847,-0.
4987194234,6.3877175012\C,1.1592184004,-1.4389797141,4.531247063\H,2.0
63978865,-1.8641784067,4.9725342634\C,0.8369510599,-1.6781246632,3.170
7619493\C,-0.3607975558,-1.1104431398,2.6642891292\H,-0.6471200511,-1.
2563078529,1.6193677373\C,-1.1818764103,-0.3336673895,3.4772889235\H,-
2.0910080112,0.1022022382,3.050863107\C,1.7346779162,-2.4877720368,2.3
367466851\C,3.0307061219,-2.9840704286,2.9092756852\H,3.7204914907,-3.
3197061151,2.1236646323\H,2.8474153916,-3.8258644017,3.6006465217\H,3.
510628279,-2.179611337,3.4868696705\N,1.4180260578,-2.7627175612,1.084
0668107\H,0.5664142926,-2.31860371,0.6154507535\C,2.1389962502,-3.6123
512175,0.1823560853\C,2.4359775179,-3.1249009192,-1.1037939824\H,2.142
6574357,-2.1148435791,-1.4029337988\C,3.1228698719,-3.9483988815,-2.00
52601442\H,3.3672902628,-3.5612773484,-2.9999435028\C,3.4986477652,-5.
2502233614,-1.638539936\C,3.173288782,-5.7378013746,-0.3624422118\H,3.
4445753358,-6.7593282506,-0.0759896243\C,2.488803112,-4.9255523785,0.5
51014429\H,2.2105874485,-5.3112801927,1.535916618\C,3.3574813722,1.049
6078528,-0.5221976421\C,3.8820766371,0.6171273141,-1.7648178795\C,3.81
33037978,0.4648578409,0.6883645237\C,4.8433702185,-0.4131956559,-1.774
0880534\C,4.7797271731,-0.5540322703,0.6330473451\C,5.3007424794,-1.01
73989861,-0.5905585388\H,5.2323858632,-0.7629238558,-2.7384472369\H,5.
1287889563,-1.0034495867,1.5706543669\C,-4.0422033474,-0.3715952492,-0
.93176383\C,-4.2439433849,-1.6877463165,-0.4441989481\C,-4.4757656684,
-0.0220040175,-2.23750141\C,-4.8877849299,-2.6286176159,-1.2703109744\
C,-5.1126323678,-0.9944206736,-3.0292151972\C,-5.3318232431,-2.3046804
372,-2.5644701541\H,-5.0403127902,-3.6466576615,-0.8904703152\H,-5.451
247875,-0.7173306478,-4.035527591\H,4.0355422138,-5.8879162062,-2.3487
788629\C,-1.7348499764,0.7905369911,5.6834699971\H,-2.803088998,0.5594
643122,5.5276926166\H,-1.4973498997,0.687292941,6.7549605809\H,-1.5936
724284,1.8509620385,5.4006266169\C,-4.2514305334,1.372187681,-2.780680
954\H,-3.1760422211,1.5471962801,-2.9686362199\C,-3.7234763064,-2.1051
234165,0.9133792143\C,-5.9947651326,-3.3402812992,-3.4460684157\H,-6.4
26078201,-4.1627788767,-2.849975659\C,6.2928701293,-2.1588417764,-0.62
10228897\H,6.6597440321,-2.3492514885,-1.6436977409\C,3.3756545,1.1994
687316,-3.065533961\H,3.522494415,2.2931117325,-3.1124531776\C,3.25277
58092,0.9160828036,2.0191222363\H,2.1855866063,0.6444731169,2.10728233
77\H,-4.0946718188,-1.4538681333,1.7232781316\H,-4.7929250137,1.520997
9015,-3.7298269317\H,-4.5831369161,2.146494748,-2.0656428727\H,-6.7978
06258,-2.8945925833,-4.0592879214\H,-5.2622090159,-3.7874543359,-4.145
8007235\H,-4.0136105911,-3.1435800729,1.1457399925\H,-2.620832606,-2.0
443464438,0.9154533097\H,7.1653097059,-1.9530108279,0.0262097755\H,5.8
285797651,-3.0921608477,-0.2499486333\H,3.892931698,0.7461038806,-3.92
80518464\H,2.293546509,0.999192698,-3.1625821111\H,3.7944905462,0.4502
560301,2.8591103921\H,3.3149641322,2.013378366,2.1334561607\\Version=E
S64L-G09RevD.01\State=1-A\HF=-2744.5738521\RMSD=5.533e-09\RMSF=4.297e-
06\Dipole=1.9357807,-1.8507178,5.1028764\Quadrupole=-5.3970991,8.00075
3,-2.6036539,-20.8029182,2.3839022,-6.5868824\PG=C01 [X(C53H48N1O4P1)]
\\@

TRIM/1E Type II

1\1\GINC-WORKER0\FOpt\RTPSSTPSS\def2SVP\C53H48N1O4P1\JHIOE\19-Feb-2019
\0\\#p tpsstpss/def2svp empiricaldispersion=gd3 int=ultrafine opt scrf
=(smd,solvent=ch2cl2,read)\\title\\0,1\P,0.2435317475,-0.5269533003,-1
.3378371932\O,-1.3323487876,-0.1477418071,-1.7685757054\O,0.4699021972
,0.6376544369,-0.117007209\O,1.0960184283,-0.2617512622,-2.5438422821\
O,0.2959534707,-1.8258336027,-0.5385430013\C,-2.2746832892,1.226493583
5,-0.047677137\C,-2.2773858888,0.0321480603,-0.7756252488\C,-3.2471058
074,-0.9997039478,-0.5809999831\C,-4.2152945273,-0.8056545488,0.395002
1261\H,-4.9823699696,-1.5717223468,0.5524632722\C,-4.2209376288,0.3501
188667,1.2262881953\C,-3.225216969,1.3750918933,1.0268646148\C,-3.1934
6662,2.4692479859,1.9443982728\H,-2.4173230832,3.2323805375,1.83842853
67\C,-4.1146485351,2.5660998959,2.9772334299\H,-4.0613104839,3.4096361
667,3.6742146243\C,-5.121032943,1.5768782932,3.1444291675\H,-5.8471699

375,1.6686300398,3.959406921\C,-5.1677743596,0.490454057,2.2856082821\
H,-5.9232767536,-0.2925053324,2.4172527029\C,-1.261439767,2.2777622615
,-0.3533282494\C,0.0983997351,1.9471696664,-0.3419123043\C,1.137467880
5,2.9186467402,-0.4742520895\C,0.7708376939,4.2406915359,-0.688774965\
H,1.5474775973,5.008387768,-0.7766670916\C,-0.5947547522,4.6274142175,
-0.8167345806\C,-1.6319984655,3.6360492501,-0.661695962\C,-2.988067127
4,4.0426678655,-0.8498283197\H,-3.7833449153,3.2953549778,-0.775682668
\C,-3.3065011483,5.3611282579,-1.1392614848\H,-4.354007383,5.646787500
3,-1.2860433405\C,-2.2857042932,6.3426535443,-1.2564074654\H,-2.551165
2176,7.3816816952,-1.4801307245\C,-0.957496745,5.9783557503,-1.1027315
506\H,-0.1597292807,6.7224823159,-1.2082502562\C,5.4833263034,-2.14012
29787,-1.1443327532\C,5.7306421425,-2.8473179851,0.0522098605\H,6.6365
427024,-3.4572612938,0.140047481\C,4.838970088,-2.7893630703,1.1275472
916\H,5.0525639248,-3.3668641124,2.0319307739\C,3.6499755476,-2.027028
9312,1.0291316133\C,3.4173557768,-1.2912790454,-0.1566097527\H,2.56956
08405,-0.6079006844,-0.2168799366\C,4.311356835,-1.35684245,-1.2226122
605\H,4.096493846,-0.775685716,-2.1241443928\C,2.6888004543,-2.0092236
362,2.1414654481\C,3.1842586652,-2.1621662917,3.5478839498\H,2.4700187
721,-1.7501644495,4.2766823964\H,4.1573633458,-1.6581790304,3.65337519
65\H,3.333581244,-3.2323566559,3.7814766065\N,1.4108029046,-1.85027446
87,1.8706826158\H,1.0758599268,-1.7875177642,0.8447980496\C,0.31534386
57,-1.8382452193,2.7946267404\C,-0.6331019434,-0.8060578198,2.67253913
84\H,-0.4958150426,-0.0350402665,1.9100882794\C,-1.7429072914,-0.79154
79705,3.5266631533\H,-2.4739474544,0.0180946614,3.443952387\C,-1.92373
29882,-1.8128813717,4.472948404\C,-0.9900559545,-2.8571649464,4.564082
8742\H,-1.1370215966,-3.6679141932,5.2853058165\C,0.1329950313,-2.8770
53562,3.7255947437\H,0.8457036435,-3.7048113935,3.7730874932\C,2.57217
12299,2.5107711645,-0.3407121448\C,3.401556444,2.4279319575,-1.4861961
731\C,3.1002132823,2.2187172891,0.9446881804\C,4.7534919051,2.06716884
75,-1.3224768813\C,4.4548225242,1.8624976753,1.0613766709\C,5.30138742
58,1.7820671853,-0.0602565273\H,5.390347601,1.9914610335,-2.2125268322
\H,4.8578875781,1.6338434849,2.0560987318\C,-3.2160576671,-2.243669579
2,-1.4118260971\C,-2.8299770476,-3.4773063639,-0.8233985007\C,-3.58450
36268,-2.1906600723,-2.7793020362\C,-2.8242400561,-4.6365252919,-1.618
9340461\C,-3.5655293993,-3.3770693425,-3.538025964\C,-3.1905104272,-4.
61074573,-2.9786059461\H,-2.5154407823,-5.5866750662,-1.1647402013\H,-
3.8534471233,-3.3321384655,-4.5958293755\H,-2.7990717664,-1.8001211591
,5.1309162534\C,6.4543043622,-2.1752093848,-2.2972938392\H,6.901453801
1,-1.1750217474,-2.4521108064\H,7.2711211387,-2.894557594,-2.123260083
3\H,5.9401721209,-2.4446147531,-3.23762474\C,-3.9858706027,-0.88263478
51,-3.4247287779\H,-3.1162056716,-0.2047077481,-3.5027870211\C,-2.3845
588995,-3.5414921068,0.6214908212\C,-3.1797698382,-5.879398954,-3.8032
646024\H,-2.1963757235,-6.381849568,-3.7499755494\C,6.7409265654,1.345
3871767,0.0926836608\H,7.3105145598,1.4908840155,-0.8407242904\C,2.832
8134937,2.65292794,-2.8697324635\H,2.3706978268,3.65082819,-2.97022757
25\C,2.2176821247,2.268198748,2.1723583253\H,1.4473667371,1.4768073419
,2.131711857\H,-3.2056148452,-3.2997725502,1.3196980058\H,7.2489790231
,1.9031614041,0.9002481813\H,6.7950936194,0.2723080333,0.3578110273\H,
2.8074195659,2.1214195987,3.0927319637\H,1.6829617781,3.2318586091,2.2
518107812\H,3.6170677866,2.5576748417,-3.6397544227\H,2.0485128537,1.9
003627647,-3.0725255495\H,-3.404337333,-5.674878539,-4.8637034339\H,-3
.9290812658,-6.6032508668,-3.4304449221\H,-4.3855651684,-1.0454863959,
-4.4397324074\H,-4.7538916732,-0.3559334004,-2.8298514312\H,-2.0092729
934,-4.5475773895,0.8738884663\H,-1.5760020982,-2.812302817,0.79703416
08\\Version=ES64L-G09RevD.01\State=1-A\HF=-2744.5726292\RMSD=2.951e-09
\RMSF=2.887e-06\Dipole=2.4766682,-1.5582316,4.8253892\Quadrupole=14.52
75706,-5.9773321,-8.5502385,-18.0566483,2.3442691,-15.847193\PG=C01 [X
(C53H48N1O4P1)]\\@

TRIM/1E Switching TS

1\1\GINC-LOGIN\SP\RTPSSTPSS\def2SVP\C53H48N1O4P1\JHIOE\29-Mar-2019\0\\
#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(smd,so
lvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,0.347012
,-0.056312,-0.132915\O,0,-0.8194,1.046381,0.395644\O,0,-0.668745,-1.30
9898,-0.619532\O,0,1.163112,-0.431289,1.083694\O,0,1.052533,0.416998,-
1.389137\C,0,-2.946032,0.281851,-0.415818\C,0,-1.949621,1.264503,-0.36
8658\C,0,-2.085861,2.528892,-1.022799\C,0,-3.222739,2.752256,-1.788624
\H,0,-3.354435,3.719799,-2.285454\C,0,-4.22022,1.750685,-1.96306\C,0,-
4.081593,0.488909,-1.278635\C,0,-5.068874,-0.516706,-1.512874\H,0,-4.9
5947,-1.493491,-1.033429\C,0,-6.150728,-0.277409,-2.347088\H,0,-6.8912
62,-1.06728,-2.514845\C,0,-6.303621,0.979797,-2.991572\H,0,-7.166332,1
.158216,-3.642726\C,0,-5.351757,1.969675,-2.805804\H,0,-5.447543,2.937
579,-3.311058\C,0,-2.797116,-0.951281,0.40804\C,0,-1.646416,-1.731182,
0.262026\C,0,-1.458557,-2.975663,0.939812\C,0,-2.457905,-3.401042,1.80
6001\H,0,-2.351361,-4.361161,2.322682\C,0,-3.616893,-2.613052,2.061077
\C,0,-3.789386,-1.358426,1.370237\C,0,-4.927034,-0.558948,1.697152\H,0

,-5.051044,0.414622,1.214188\C,0,-5.863523,-0.992075,2.624085\H,0,-6.7
25085,-0.358479,2.862143\C,0,-5.712084,-2.246915,3.273633\H,0,-6.46228
2,-2.580411,3.998989\C,0,-4.606352,-3.03591,2.999637\H,0,-4.465903,-3.
996337,3.508803\C,0,-0.237275,-3.803668,0.687657\C,0,0.776864,-3.90790
5,1.676037\C,0,-0.10901,-4.500115,-0.539959\C,0,1.906551,-4.701811,1.4
08065\C,0,1.030429,-5.297531,-0.757943\C,0,2.054769,-5.406285,0.198392
\H,0,2.698138,-4.765781,2.165529\H,0,1.11932,-5.84353,-1.705373\C,0,-1
.063898,3.607726,-0.836329\C,0,-0.112245,3.883085,-1.850966\C,0,-1.083
45,4.378063,0.353216\C,0,0.807708,4.929139,-1.651564\C,0,-0.155075,5.4
25578,0.504643\C,0,0.802564,5.715401,-0.483985\H,0,1.552152,5.133096,-
2.431437\H,0,-0.172304,6.0193,1.427014\C,0,-2.070995,4.065463,1.455446
\H,0,-1.875115,3.063586,1.880803\C,0,-0.05916,3.039217,-3.104875\C,0,1
.83792,6.798274,-0.276282\H,0,2.818032,6.353849,-0.015613\C,0,3.301895
,-6.216979,-0.075022\H,0,3.532767,-6.900737,0.761976\C,0,0.682375,-3.1
29948,2.969749\H,0,-0.229323,-3.382758,3.539211\C,0,-1.167519,-4.37968
8,-1.613991\H,0,-1.166843,-3.361028,-2.043893\H,0,-1.027942,3.036937,-
3.635568\C,0,3.140834,3.620855,2.786681\C,0,4.329843,2.952414,3.148093
\H,0,4.8669,3.255577,4.053427\C,0,4.833401,1.903037,2.374798\H,0,5.747
57,1.398858,2.699477\C,0,4.152672,1.476197,1.208129\C,0,2.964809,2.159
26,0.836006\H,0,2.435748,1.894154,-0.085368\C,0,2.47287,3.201691,1.614
503\H,0,1.557825,3.712501,1.30136\C,0,4.657005,0.372943,0.386862\C,0,6
.091485,-0.046117,0.445774\H,0,6.418433,-0.091579,1.497112\H,0,6.72562
3,0.706387,-0.056601\H,0,6.254765,-1.027074,-0.022288\N,0,3.802075,-0.
239926,-0.412088\H,0,2.790923,-0.020217,-0.295224\C,0,4.050581,-1.2045
42,-1.433453\C,0,5.074223,-1.016606,-2.380772\H,0,5.704745,-0.124159,-
2.340972\C,0,5.24954,-1.966413,-3.395697\H,0,6.042364,-1.822151,-4.136
967\C,0,4.403256,-3.08369,-3.473159\C,0,3.372155,-3.249814,-2.534329\H
,0,2.705328,-4.114723,-2.59327\C,0,3.186153,-2.312395,-1.51146\H,0,2.3
92023,-2.44065,-0.769892\H,0,4.53996,-3.820831,-4.2713\C,0,2.592378,4.
765222,3.599978\H,0,3.152732,4.907779,4.538175\H,0,2.639969,5.706864,3
.020565\H,0,1.527809,4.596686,3.843477\H,0,1.555307,-3.330388,3.61393\
H,0,0.650908,-2.048068,2.74636\H,0,3.200887,-6.816732,-0.995306\H,0,4.
179015,-5.55393,-0.200795\H,0,-2.003531,4.803716,2.272054\H,0,-3.11022
7,4.055715,1.079668\H,0,0.713565,3.409795,-3.799855\H,0,0.178815,1.992
656,-2.839105\H,0,1.989383,7.39648,-1.192536\H,0,1.553101,7.48075,0.54
2539\H,0,-0.987261,-5.09625,-2.432772\H,0,-2.180584,-4.558621,-1.21092
4\\Version=ES64L-G09RevD.01\State=1-A\HF=-2744.5365861\RMSD=5.105e-09\
Dipole=4.9306913,0.7434514,0.6187754\Quadrupole=33.8890338,-12.5399608
,-21.349073,3.2576982,1.1289285,12.9675487\PG=C01 [X(C53H48N1O4P1)]\\@

TRIP/1E Type II

Conf0

1\1\GINC-WORKER0\SP\RTPSSTPSS\def2SVP\C65H72N1O4P1\JHIOE\05-May-2019\0
\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(smd,
solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,-0.211
306,-0.543612,-1.05158\O,0,-1.540091,0.439014,-1.327676\O,0,0.72606,0.
529948,-0.118359\O,0,0.385891,-0.829223,-2.396274\O,0,-0.547219,-1.626
422,-0.030592\C,0,-1.478252,2.243368,0.238585\C,0,-2.112545,1.104448,-
0.262652\C,0,-3.368933,0.626001,0.22375\C,0,-3.958837,1.315777,1.27395
4\H,0,-4.934559,0.993605,1.651432\C,0,-3.316655,2.423498,1.898685\C,0,
-2.049237,2.891538,1.393179\C,0,-1.388242,3.943195,2.097643\H,0,-0.405
365,4.279643,1.755322\C,0,-1.961277,4.523334,3.220465\H,0,-1.428719,5.
320343,3.750891\C,0,-3.227744,4.086329,3.693607\H,0,-3.671901,4.55561,
4.578195\C,0,-3.887699,3.05469,3.044385\H,0,-4.854138,2.691907,3.41240
1\C,0,-0.212075,2.72164,-0.386198\C,0,0.874696,1.847981,-0.499038\C,0,
2.180442,2.281763,-0.890914\C,0,2.339154,3.604938,-1.278893\H,0,3.3311
92,3.965002,-1.571016\C,0,1.239185,4.510508,-1.319892\C,0,-0.058969,4.
071167,-0.868889\C,0,-1.149475,4.989465,-0.949817\H,0,-2.147298,4.6607
72,-0.644502\C,0,-0.963586,6.28056,-1.421893\H,0,-1.817054,6.964956,-1
.481725\C,0,0.322065,6.720762,-1.836525\H,0,0.45617,7.74472,-2.202098\
C,0,1.398728,5.849143,-1.788784\H,0,2.392434,6.172002,-2.1198\C,0,3.55
0461,-4.331604,-1.369587\C,0,3.504131,-5.127359,-0.204594\H,0,3.902079
,-6.147731,-0.231619\C,0,2.963616,-4.634861,0.986739\H,0,2.932985,-5.2
77792,1.871777\C,0,2.4182,-3.33021,1.037007\C,0,2.478781,-2.522418,-0.
122918\H,0,2.154709,-1.479998,-0.082659\C,0,3.033534,-3.020473,-1.3013
42\H,0,3.080199,-2.369575,-2.178535\C,0,1.830766,-2.824969,2.287924\C,
0,2.467037,-3.194444,3.593188\H,0,2.267833,-2.440306,4.370141\H,0,3.55
2801,-3.308125,3.453202\H,0,2.069053,-4.163289,3.948083\N,0,0.77992,-2
.037666,2.208018\H,0,0.33831,-1.849618,1.235057\C,0,0.061755,-1.39607,
3.263479\C,0,-0.351154,-0.068852,3.034427\H,0,-0.097396,0.41785,2.0887
21\C,0,-1.077239,0.606113,4.022743\H,0,-1.383219,1.64216,3.851368\C,0,
-1.417362,-0.04301,5.220411\C,0,-1.033615,-1.377385,5.426056\H,0,-1.31
7798,-1.898061,6.346438\C,0,-0.295495,-2.062354,4.450965\H,0,-0.036356
,-3.113063,4.598809\C,0,3.336628,1.33234,-0.800761\C,0,3.915921,0.7755
77,-1.968791\C,0,3.850003,0.993892,0.484423\C,0,5.003799,-0.110133,-1.

828311\C,0,4.935727,0.107662,0.569663\C,0,5.525536,-0.462006,-0.574498
\H,0,5.452257,-0.550665,-2.726998\H,0,5.333994,-0.149227,1.55639\C,0,-
4.027711,-0.556554,-0.418635\C,0,-4.140596,-1.788724,0.281067\C,0,-4.5
56491,-0.436036,-1.73424\C,0,-4.820243,-2.856965,-0.336704\C,0,-5.2153
41,-1.536361,-2.309187\C,0,-5.368139,-2.755254,-1.625233\H,0,-4.919699
,-3.807524,0.200857\H,0,-5.62568,-1.434712,-3.320788\H,0,-1.9926,0.487
458,5.986459\C,0,4.183327,-4.834289,-2.642924\H,0,5.148579,-4.32093,-2
.816551\H,0,4.377135,-5.91883,-2.603884\H,0,3.544212,-4.618103,-3.5172
93\C,0,-4.446235,0.859632,-2.540603\H,0,-3.879719,1.589296,-1.938393\C
,0,-3.535912,-1.994504,1.672265\C,0,-6.101618,-3.933163,-2.261641\H,0,
-6.057279,-4.770799,-1.540158\C,0,-4.619082,-1.953399,2.770682\H,0,-4.
161227,-2.066325,3.770652\H,0,-5.177649,-1.001479,2.757559\H,0,-5.3486
15,-2.774026,2.636064\C,0,-5.416272,-4.40016,-3.562365\H,0,-5.442756,-
3.609819,-4.33503\H,0,-4.358689,-4.664757,-3.384253\H,0,-5.928636,-5.2
89346,-3.973679\C,0,-7.589252,-3.606155,-2.507415\H,0,-8.120146,-4.486
754,-2.913639\H,0,-8.092262,-3.303874,-1.571371\H,0,-7.701305,-2.78035
7,-3.234143\C,0,-3.662705,0.645066,-3.851851\H,0,-4.198502,-0.038602,-
4.536188\H,0,-3.525028,1.606874,-4.379728\H,0,-2.665932,0.220389,-3.64
439\C,0,-5.835215,1.477034,-2.805138\H,0,-5.736264,2.43928,-3.340548\H
,0,-6.4627,0.809889,-3.424663\H,0,-6.373232,1.666264,-1.858714\C,0,6.7
07782,-1.420808,-0.461291\H,0,6.840794,-1.886749,-1.456082\C,0,3.40372
5,1.123251,-3.367957\H,0,2.4598,1.681642,-3.244981\C,0,3.281127,1.6374
82,1.751527\H,0,2.220706,1.873564,1.558832\C,0,8.005338,-0.654974,-0.1
25241\H,0,8.869421,-1.343745,-0.086424\H,0,8.218831,0.121627,-0.881304
\H,0,7.923498,-0.15651,0.858572\C,0,6.453175,-2.55077,0.555718\H,0,6.3
7807,-2.158554,1.586606\H,0,5.51717,-3.089141,0.327836\H,0,7.282708,-3
.281056,0.538706\C,0,3.319578,0.719135,2.984891\H,0,2.861568,-0.259489
,2.76661\H,0,4.351001,0.542264,3.340324\H,0,2.759441,1.179705,3.817786
\C,0,4.001815,2.973567,2.036521\H,0,3.916828,3.664013,1.178903\H,0,3.5
67086,3.472076,2.922605\H,0,5.076773,2.80233,2.230821\C,0,4.401928,2.0
47031,-4.097492\H,0,4.600291,2.964729,-3.515343\H,0,5.368941,1.535934,
-4.261762\H,0,4.005252,2.347442,-5.084867\C,0,3.078029,-0.12767,-4.207
067\H,0,2.698085,0.17316,-5.201039\H,0,3.970649,-0.758532,-4.372067\H,
0,2.296329,-0.72408,-3.708653\C,0,-2.71952,-3.299364,1.764291\H,0,-3.3
61215,-4.194437,1.668865\H,0,-1.949162,-3.32764,0.97716\H,0,-2.215962,
-3.359542,2.745531\H,0,-2.835701,-1.161555,1.852915\\Version=ES64L-G09
RevD.01\State=1-A\HF=-3216.0970767\RMSD=2.351e-09\Dipole=2.3432935,-1.
9836445,4.6565248\Quadrupole=-8.428126,9.3776108,-0.9494848,-19.947016
2,-2.2136709,-12.9820098\PG=C01 [X(C65H72N1O4P1)]\\@

Conf1

1\1\GINC-WORKER2\SP\RTPSSTPSS\def2SVP\C65H72N1O4P1\JHIOE\05-May-2019\0
\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(smd,
solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,-0.199
09,-0.47727,-1.120182\O,0,-1.493382,0.546728,-1.409092\O,0,0.738125,0.
544853,-0.130925\O,0,0.430098,-0.740852,-2.454853\O,0,-0.592234,-1.575
552,-0.136942\C,0,-1.424315,2.31929,0.191846\C,0,-2.075827,1.207383,-0
.346734\C,0,-3.356371,0.754095,0.099124\C,0,-3.956484,1.443786,1.14378
2\H,0,-4.950319,1.142061,1.489607\C,0,-3.302904,2.524301,1.803354\C,0,
-2.009656,2.965057,1.340575\C,0,-1.340308,3.986777,2.080209\H,0,-0.339
754,4.3017,1.770546\C,0,-1.92831,4.564732,3.196311\H,0,-1.389153,5.338
473,3.753867\C,0,-3.218763,4.155427,3.627449\H,0,-3.674264,4.622937,4.
507195\C,0,-3.888327,3.152988,2.943267\H,0,-4.874369,2.81166,3.27843\C
,0,-0.125295,2.768972,-0.385262\C,0,0.938511,1.865297,-0.476927\C,0,2.
270116,2.266493,-0.811345\C,0,2.482726,3.590885,-1.167809\H,0,3.495238
,3.926542,-1.415386\C,0,1.411497,4.528983,-1.234056\C,0,0.085318,4.120
948,-0.838447\C,0,-0.975039,5.071284,-0.944364\H,0,-1.992182,4.765803,
-0.681369\C,0,-0.735513,6.363093,-1.389523\H,0,-1.566425,7.072636,-1.4
70559\C,0,0.576812,6.772069,-1.749081\H,0,0.753434,7.796949,-2.093458\
C,0,1.626189,5.869482,-1.674893\H,0,2.640195,6.168766,-1.963898\C,0,3.
352282,-4.410132,-1.484189\C,0,2.920414,-3.072292,-1.386051\H,0,3.0053
83,-2.406863,-2.248915\C,0,2.392707,-2.56762,-0.195839\H,0,2.129952,-1
.509049,-0.131729\C,0,2.277042,-3.396114,0.942768\C,0,2.747109,-4.7299
44,0.865655\H,0,2.676607,-5.388547,1.736857\C,0,3.259185,-5.226917,-0.
334474\H,0,3.59397,-6.269079,-0.384656\C,0,1.698308,-2.891416,2.198207
\C,0,2.303971,-3.315133,3.501411\H,0,2.134998,-2.566538,4.290897\H,0,3
.383905,-3.480312,3.368251\H,0,1.854212,-4.269105,3.834232\N,0,0.67929
8,-2.06285,2.121891\H,0,0.259703,-1.843133,1.146046\C,0,-0.033516,-1.4
17187,3.178793\C,0,-0.413255,-0.078217,2.960163\H,0,-0.136634,0.412282
,2.02306\C,0,-1.135192,0.603624,3.946669\H,0,-1.416115,1.647876,3.7813
29\C,0,-1.503339,-0.049355,5.133863\C,0,-1.152084,-1.394118,5.32975\H,
0,-1.458359,-1.917253,6.241608\C,0,-0.419613,-2.086752,4.355759\H,0,-0
.18758,-3.144523,4.497316\C,0,3.390655,1.278157,-0.693354\C,0,3.989424
,0.714096,-1.847492\C,0,3.847034,0.907937,0.604996\C,0,5.042567,-0.208
894,-1.681119\C,0,4.899189,-0.014709,0.715904\C,0,5.510149,-0.589983,-
0.414792\H,0,5.507701,-0.65291,-2.569513\H,0,5.256617,-0.295433,1.7120
3\C,0,-4.027843,-0.404248,-0.574097\C,0,-4.188562,-1.641986,0.110594\C

,0,-4.522483,-0.25728,-1.89793\C,0,-4.882465,-2.68461,-0.529308\C,0,-5
.198635,-1.336804,-2.497532\C,0,-5.399886,-2.555336,-1.830436\H,0,-5.0
13604,-3.63406,0.00196\H,0,-5.586546,-1.223177,-3.517466\H,0,-2.07496,
0.486186,5.899092\C,0,3.951983,-4.940453,-2.762547\H,0,3.643269,-5.983
539,-2.950038\H,0,3.666052,-4.322007,-3.629547\H,0,5.05746,-4.93469,-2
.697134\C,0,-4.36083,1.042265,-2.68854\H,0,-3.794236,1.75292,-2.063997
\C,0,-3.615395,-1.87779,1.510554\C,0,-6.147638,-3.704197,-2.501537\H,0
,-6.432486,-3.358679,-3.51322\C,0,-4.716905,-1.818021,2.589583\H,0,-4.
281007,-1.951888,3.596737\H,0,-5.250276,-0.851892,2.575479\H,0,-5.4648
78,-2.618067,2.43362\C,0,-7.444704,-4.052129,-1.74222\H,0,-7.223268,-4
.413566,-0.720964\H,0,-8.10433,-3.170206,-1.65394\H,0,-8.004245,-4.848
343,-2.266918\C,0,-5.250143,-4.947831,-2.666207\H,0,-5.788112,-5.74864
9,-3.206215\H,0,-4.333707,-4.706371,-3.233745\H,0,-4.943415,-5.351482,
-1.683686\C,0,-3.547055,0.821679,-3.980108\H,0,-4.078354,0.154964,-4.6
84317\H,0,-3.375644,1.784719,-4.495736\H,0,-2.565158,0.374875,-3.74958
3\C,0,-5.727319,1.694553,-2.983577\H,0,-5.591686,2.658743,-3.507382\H,
0,-6.354258,1.048228,-3.625194\H,0,-6.284979,1.88853,-2.04953\C,0,6.65
1025,-1.593172,-0.266641\H,0,6.88578,-1.96838,-1.280715\C,0,3.543654,1
.104634,-3.258104\H,0,2.606847,1.680023,-3.160936\C,0,3.255191,1.55709
6,1.85877\H,0,2.20582,1.815804,1.636454\C,0,7.922009,-0.91716,0.289368
\H,0,8.757536,-1.63927,0.341885\H,0,8.238142,-0.072188,-0.348152\H,0,7
.748858,-0.526487,1.309317\C,0,6.245798,-2.804101,0.598061\H,0,6.03043
5,-2.502271,1.639714\H,0,5.344499,-3.296725,0.195563\H,0,7.061178,-3.5
50009,0.627912\C,0,3.239935,0.634618,3.089866\H,0,2.765935,-0.333718,2
.85926\H,0,4.257406,0.434845,3.47231\H,0,2.668291,1.106443,3.908528\C,
0,3.995043,2.876558,2.17187\H,0,3.951532,3.572624,1.315793\H,0,3.54405
1,3.380381,3.046742\H,0,5.059557,2.681045,2.397962\C,0,4.592194,2.0244
09,-3.919266\H,0,4.784747,2.92179,-3.304589\H,0,5.554067,1.49548,-4.05
4675\H,0,4.24521,2.35878,-4.914401\C,0,3.22864,-0.115298,-4.145017\H,0
,2.902987,0.221482,-5.146634\H,0,4.112511,-0.764049,-4.285965\H,0,2.40
9626,-0.704467,-3.70085\C,0,-2.837292,-3.205864,1.60331\H,0,-3.501951,
-4.081497,1.486555\H,0,-2.053997,-3.247816,0.829682\H,0,-2.353935,-3.2
90421,2.592826\H,0,-2.895582,-1.066727,1.712255\\Version=ES64L-G09RevD
.01\State=1-A\HF=-3216.0970674\RMSD=2.411e-09\Dipole=2.1511303,-2.2072
221,4.6778427\Quadrupole=-9.8259229,12.0811125,-2.2551896,-18.9268475,
-3.0530027,-12.2754142\PG=C01 [X(C65H72N1O4P1)]\\@

Conf2

1\1\GINC-WORKER0\SP\RTPSSTPSS\def2SVP\C65H72N1O4P1\JHIOE\05-May-2019\0
\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(smd,
solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,-0.155
228,-0.579395,-0.967524\O,0,-1.438658,0.42075,-1.366627\O,0,0.754101,0
.513805,-0.029774\O,0,0.513917,-0.942732,-2.258201\O,0,-0.587418,-1.60
3041,0.077683\C,0,-1.442528,2.273002,0.141688\C,0,-2.06485,1.127965,-0
.360351\C,0,-3.355556,0.682816,0.064064\C,0,-3.997133,1.417735,1.05174
6\H,0,-4.999718,1.124407,1.378874\C,0,-3.376638,2.537694,1.676662\C,0,
-2.073467,2.970274,1.234824\C,0,-1.441817,4.038812,1.94066\H,0,-0.4350
51,4.34979,1.648056\C,0,-2.074505,4.668043,3.003484\H,0,-1.563772,5.47
7591,3.536325\C,0,-3.373777,4.26429,3.412975\H,0,-3.864271,4.77124,4.2
51036\C,0,-4.007391,3.21744,2.761794\H,0,-4.999691,2.880162,3.082335\C
,0,-0.134269,2.709553,-0.424584\C,0,0.941952,1.814709,-0.45113\C,0,2.2
70396,2.212857,-0.799977\C,0,2.471272,3.521275,-1.218696\H,0,3.482306,
3.854152,-1.47594\C,0,1.393297,4.445004,-1.337501\C,0,0.066365,4.03988
8,-0.942596\C,0,-1.001988,4.972788,-1.109781\H,0,-2.020526,4.668775,-0
.851344\C,0,-0.768606,6.24621,-1.607759\H,0,-1.605769,6.941729,-1.7335
18\C,0,0.544994,6.654106,-1.964138\H,0,0.716416,7.664687,-2.350753\C,0
,1.601508,5.766428,-1.835488\H,0,2.616792,6.062514,-2.12326\C,0,3.3800
33,-4.498677,-0.906033\C,0,2.9726,-3.150063,-0.884041\H,0,3.138571,-2.
516376,-1.759657\C,0,2.373378,-2.594182,0.248702\H,0,2.128611,-1.52925
7,0.256458\C,0,2.163234,-3.379228,1.4049\C,0,2.604879,-4.725187,1.4047
02\H,0,2.458762,-5.351126,2.290671\C,0,3.18613,-5.273761,0.26038\H,0,3
.500474,-6.323492,0.268332\C,0,1.521772,-2.812329,2.602018\C,0,2.03259
,-3.190567,3.958784\H,0,1.852763,-2.390769,4.69428\H,0,3.109442,-3.409
324,3.902064\H,0,1.519917,-4.102952,4.316322\N,0,0.534941,-1.96088,2.4
26616\H,0,0.175942,-1.785633,1.416753\C,0,-0.21323,-1.238951,3.405937\
C,0,-0.522414,0.101418,3.1021\H,0,-0.166834,0.535963,2.16361\C,0,-1.27
8039,0.855422,4.00759\H,0,-1.504575,1.900551,3.778827\C,0,-1.750818,0.
273151,5.194446\C,0,-1.46658,-1.072443,5.474595\H,0,-1.853256,-1.53970
5,6.386283\C,0,-0.699195,-1.836435,4.584427\H,0,-0.51618,-2.893487,4.7
88585\C,0,3.417597,1.259815,-0.647689\C,0,4.039479,0.687945,-1.788694\
C,0,3.906187,0.965319,0.655219\C,0,5.165107,-0.13767,-1.605589\C,0,5.0
34339,0.135074,0.784315\C,0,5.687539,-0.41705,-0.33139\H,0,5.648612,-0
.57182,-2.488369\H,0,5.428801,-0.084659,1.783075\C,0,-3.992199,-0.5131
01,-0.576324\C,0,-4.176093,-1.71483,0.160919\C,0,-4.428565,-0.437254,-
1.928834\C,0,-4.838244,-2.793398,-0.45754\C,0,-5.069459,-1.548562,-2.5
03418\C,0,-5.296624,-2.734295,-1.78317\H,0,-4.992347,-3.719527,0.10895
1\H,0,-5.404763,-1.482562,-3.545152\H,0,-2.350516,0.865497,5.893445\C,

0,4.044046,-5.094083,-2.122536\H,0,3.496121,-5.987742,-2.473542\H,0,4.
095451,-4.368036,-2.94997\H,0,5.072992,-5.421324,-1.883397\C,0,-4.2410
03,0.821196,-2.778528\H,0,-3.707247,1.569361,-2.169105\C,0,-3.658689,-
1.880524,1.592103\C,0,-5.989846,-3.932305,-2.426483\H,0,-6.10599,-4.70
0324,-1.638714\C,0,-4.802213,-1.777047,2.62324\H,0,-4.405745,-1.853795
,3.652485\H,0,-5.342695,-0.818646,2.537555\H,0,-5.536534,-2.591929,2.4
8001\C,0,-5.123525,-4.542873,-3.547949\H,0,-4.975629,-3.822056,-4.3732
7\H,0,-4.12733,-4.832203,-3.168357\H,0,-5.606618,-5.444278,-3.968369\C
,0,-7.397789,-3.576437,-2.944915\H,0,-7.902256,-4.474182,-3.346977\H,0
,-8.028368,-3.161826,-2.138014\H,0,-7.350087,-2.827253,-3.756669\C,0,-
3.371413,0.540385,-4.021301\H,0,-3.866838,-0.16954,-4.709253\H,0,-3.18
778,1.475924,-4.581414\H,0,-2.396134,0.118589,-3.725892\C,0,-5.598815,
1.442687,-3.165234\H,0,-5.449154,2.382607,-3.727831\H,0,-6.189471,0.75
8859,-3.802499\H,0,-6.200082,1.673453,-2.267273\C,0,6.927798,-1.28999,
-0.156235\H,0,7.16665,-1.298142,0.924082\C,0,3.533673,0.964387,-3.2059
14\H,0,2.567179,1.489157,-3.115409\C,0,3.272983,1.598974,1.896123\H,0,
2.223227,1.833055,1.651385\C,0,6.663771,-2.747211,-0.586875\H,0,7.5638
43,-3.369667,-0.429419\H,0,5.834836,-3.188119,-0.007521\H,0,6.396891,-
2.803394,-1.657988\C,0,8.144554,-0.70187,-0.899101\H,0,7.981635,-0.696
785,-1.992557\H,0,8.342965,0.337318,-0.580402\H,0,9.050899,-1.302042,-
0.698073\C,0,3.251307,0.665426,3.119475\H,0,2.802298,-0.310245,2.86854
7\H,0,4.264805,0.481944,3.519907\H,0,2.653982,1.117515,3.931128\C,0,3.
972332,2.934604,2.230116\H,0,3.929303,3.631498,1.374335\H,0,3.488969,3
.424127,3.09581\H,0,5.03651,2.76724,2.479369\C,0,4.503952,1.896014,-3.
961884\H,0,4.661004,2.842682,-3.414765\H,0,5.491228,1.416118,-4.096913
\H,0,4.10649,2.141742,-4.963936\C,0,3.268215,-0.331829,-3.996825\H,0,2
.892861,-0.08725,-5.007868\H,0,4.186636,-0.934521,-4.121598\H,0,2.5013
15,-0.93652,-3.485767\C,0,-2.879221,-3.198276,1.777228\H,0,-3.535891,-
4.08198,1.677976\H,0,-2.066978,-3.273439,1.036588\H,0,-2.433127,-3.232
927,2.78703\H,0,-2.950683,-1.056251,1.781902\\Version=ES64L-G09RevD.01
\State=1-A\HF=-3216.0959114\RMSD=2.239e-09\Dipole=1.8737331,-1.9436175
,4.8971892\Quadrupole=-10.7882883,10.2639406,0.5243477,-17.931839,-2.4
719673,-14.8071693\PG=C01 [X(C65H72N1O4P1)]\\@

Conf3

1\1\GINC-WORKER2\SP\RTPSSTPSS\def2SVP\C65H72N1O4P1\JHIOE\05-May-2019\0
\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(smd,
solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,-0.216
017,-0.537977,-1.069941\O,0,-1.545208,0.445569,-1.341215\O,0,0.728224,
0.534188,-0.142033\O,0,0.375417,-0.823764,-2.417141\O,0,-0.549913,-1.6
1786,-0.045375\C,0,-1.460074,2.267169,0.202987\C,0,-2.103595,1.124232,
-0.277059\C,0,-3.354082,0.65363,0.231815\C,0,-3.929704,1.358872,1.2796
81\H,0,-4.9008,1.043347,1.674288\C,0,-3.278431,2.473956,1.881475\C,0,-
2.016074,2.932585,1.355116\C,0,-1.34481,3.991941,2.038216\H,0,-0.36520
3,4.321958,1.680605\C,0,-1.90373,4.587637,3.160051\H,0,-1.363613,5.390
35,3.673981\C,0,-3.16536,4.159423,3.65365\H,0,-3.598375,4.64079,4.5372
7\C,0,-3.834796,3.120931,3.025518\H,0,-4.797485,2.76471,3.409404\C,0,-
0.193975,2.728904,-0.434712\C,0,0.887493,1.847288,-0.534545\C,0,2.1979
39,2.268219,-0.924196\C,0,2.365036,3.584396,-1.332181\H,0,3.360407,3.9
35279,-1.624297\C,0,1.269747,4.494791,-1.391837\C,0,-0.031838,4.070158
,-0.936268\C,0,-1.116623,4.993769,-1.031009\H,0,-2.116253,4.675525,-0.
72036\C,0,-0.922821,6.275998,-1.523608\H,0,-1.771979,6.964709,-1.59448
3\C,0,0.365582,6.701533,-1.945089\H,0,0.505813,7.71848,-2.327553\C,0,1
.437265,5.824677,-1.882317\H,0,2.433035,6.136714,-2.217518\C,0,3.4111,
-4.384289,-1.449758\C,0,2.952858,-3.054539,-1.363125\H,0,3.001324,-2.4
02597,-2.238851\C,0,2.446443,-2.539442,-0.168112\H,0,2.163647,-1.48535
,-0.116669\C,0,2.379366,-3.349478,0.987916\C,0,2.87546,-4.674507,0.920
751\H,0,2.842768,-5.318682,1.804913\C,0,3.365951,-5.182145,-0.283841\H
,0,3.721797,-6.217726,-0.324495\C,0,1.826044,-2.833339,2.250151\C,0,2.
473182,-3.222961,3.543793\H,0,2.3237,-2.455353,4.319067\H,0,3.549598,-
3.385603,3.382833\H,0,2.039158,-4.170138,3.914636\N,0,0.792697,-2.0213
18,2.18778\H,0,0.341234,-1.830817,1.220107\C,0,0.104729,-1.358414,3.25
0211\C,0,-0.301171,-0.03107,3.007645\H,0,-0.063842,0.436365,2.048141\C
,0,-0.997833,0.669144,3.999363\H,0,-1.298165,1.704723,3.815293\C,0,-1.
316059,0.045572,5.216426\C,0,-0.940726,-1.288779,5.436788\H,0,-1.20859
4,-1.790187,6.372625\C,0,-0.232465,-1.999374,4.457734\H,0,0.017356,-3.
049749,4.621315\C,0,3.348211,1.31432,-0.805673\C,0,3.940484,0.737388,-
1.956992\C,0,3.842952,0.992677,0.492005\C,0,5.022453,-0.15189,-1.78888
2\C,0,4.922287,0.102411,0.604406\C,0,5.525415,-0.486755,-0.523306\H,0,
5.481701,-0.606574,-2.674989\H,0,5.308585,-0.141089,1.599504\C,0,-4.02
3718,-0.538553,-0.381813\C,0,-4.119539,-1.761472,0.336759\C,0,-4.5826,
-0.436166,-1.686292\C,0,-4.813502,-2.837467,-0.250334\C,0,-5.256883,-1
.543266,-2.229887\C,0,-5.393267,-2.752741,-1.52611\H,0,-4.898937,-3.78
1143,0.301448\H,0,-5.690782,-1.4551,-3.232914\H,0,-1.868086,0.595453,5
.985848\C,0,3.990507,-4.923636,-2.733656\H,0,3.689029,-5.972023,-2.902
768\H,0,3.680898,-4.31865,-3.601964\H,0,5.096927,-4.906188,-2.689827\C
,0,-4.4845,0.846376,-2.514792\H,0,-3.9087,1.585061,-1.932559\C,0,-3.48

2885,-1.948507,1.716044\C,0,-6.138215,-3.940819,-2.129115\H,0,-6.07947
4,-4.766401,-1.394843\C,0,-4.537279,-1.875794,2.840351\H,0,-4.054849,-
1.975356,3.830106\H,0,-5.086529,-0.918619,2.823913\H,0,-5.278381,-2.69
0982,2.739727\C,0,-5.475179,-4.428541,-3.43379\H,0,-5.516569,-3.651146
,-4.218806\H,0,-4.414142,-4.688336,-3.269654\H,0,-5.993083,-5.325376,-
3.820802\C,0,-7.630588,-3.620008,-2.352945\H,0,-8.166855,-4.507882,-2.
735567\H,0,-8.117202,-3.304161,-1.412685\H,0,-7.757833,-2.806016,-3.09
0383\C,0,-3.719795,0.608832,-3.833364\H,0,-4.265258,-0.087064,-4.49744
8\H,0,-3.590011,1.561089,-4.380223\H,0,-2.719897,0.188066,-3.633076\C,
0,-5.87656,1.46052,-2.770188\H,0,-5.784314,2.41461,-3.321105\H,0,-6.51
2317,0.784704,-3.371598\H,0,-6.402146,1.664206,-1.819788\C,0,6.691328,
-1.45997,-0.371033\H,0,6.92411,-1.846488,-1.381283\C,0,3.452427,1.0718
79,-3.36809\H,0,2.514622,1.644512,-3.26601\C,0,3.261704,1.658368,1.742
106\H,0,2.19927,1.876977,1.539959\C,0,7.952002,-0.747467,0.161711\H,0,
8.803875,-1.449966,0.217675\H,0,8.243175,0.093926,-0.492268\H,0,7.7802
96,-0.344431,1.177055\C,0,6.320232,-2.664511,0.517729\H,0,6.110784,-2.
349191,1.5566\H,0,5.423923,-3.180719,0.134475\H,0,7.150208,-3.394065,0
.550331\C,0,3.306762,0.769622,2.996773\H,0,2.871505,-0.223428,2.797831
\H,0,4.338125,0.623072,3.365899\H,0,2.72941,1.237826,3.813388\C,0,3.96
5295,3.008961,2.00063\H,0,3.877799,3.679165,1.127545\H,0,3.519254,3.52
2205,2.872555\H,0,5.04088,2.854328,2.204956\C,0,4.472802,1.972527,-4.0
96002\H,0,4.676477,2.894661,-3.522756\H,0,5.434569,1.446298,-4.241906\
H,0,4.092494,2.266147,-5.091823\C,0,3.120337,-0.185411,-4.195198\H,0,2
.766956,0.106904,-5.201402\H,0,4.003536,-0.836217,-4.33104\H,0,2.31662
3,-0.758791,-3.704731\C,0,-2.678331,-3.260246,1.8136\H,0,-3.331928,-4.
150035,1.757559\H,0,-1.931124,-3.315641,1.005929\H,0,-2.147435,-3.3040
22,2.781115\H,0,-2.769819,-1.11994,1.863624\\Version=ES64L-G09RevD.01\
State=1-A\HF=-3216.0970157\RMSD=2.389e-09\Dipole=2.3361036,-2.0319428,
4.6541888\Quadrupole=-9.4883586,10.703515,-1.2151564,-19.9919649,-1.92
95199,-12.598029\PG=C01 [X(C65H72N1O4P1)]\\@

TRIP/1E Type I

Conf0

1\1\GINC-LOGIN\SP\RTPSSTPSS\def2SVP\C65H72N1O4P1\JHIOE\06-May-2019\0\\
#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(smd,so
lvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,-0.10843
9,-0.447366,-1.242731\O,0,-1.431908,0.570095,-1.391101\O,0,0.823429,0.
472831,-0.160745\O,0,0.504533,-0.533094,-2.608759\O,0,-0.45731,-1.6674
14,-0.396129\C,0,-1.312229,2.256433,0.304329\C,0,-1.988344,1.187587,-0
.291383\C,0,-3.286663,0.753824,0.125556\C,0,-3.876454,1.410077,1.19781
\H,0,-4.878244,1.113224,1.525644\C,0,-3.198893,2.438397,1.913361\C,0,-
1.887489,2.858895,1.482717\C,0,-1.192634,3.818651,2.27983\H,0,-0.17906
7,4.115366,1.995523\C,0,-1.773362,4.360781,3.417199\H,0,-1.214585,5.08
7395,4.017267\C,0,-3.082128,3.976408,3.814797\H,0,-3.531886,4.416673,4
.711386\C,0,-3.77625,3.030518,3.07697\H,0,-4.77625,2.705804,3.386313\C
,0,-0.009473,2.720243,-0.252886\C,0,1.041097,1.811262,-0.414385\C,0,2.
374166,2.213048,-0.740573\C,0,2.602375,3.555336,-1.010021\H,0,3.617068
,3.893658,-1.244154\C,0,1.54403,4.509893,-1.004389\C,0,0.215367,4.0953
77,-0.625037\C,0,-0.833204,5.063391,-0.669616\H,0,-1.853229,4.756108,-
0.420771\C,0,-0.579725,6.376061,-1.040006\H,0,-1.402474,7.098707,-1.07
6085\C,0,0.735988,6.78997,-1.380543\H,0,0.923725,7.831021,-1.665393\C,
0,1.774135,5.871738,-1.365401\H,0,2.790502,6.174335,-1.642256\C,0,-1.4
84247,-0.672644,4.67252\C,0,-0.968356,-1.891613,5.160822\H,0,-1.320245
,-2.279614,6.123\C,0,-0.012532,-2.614593,4.439549\H,0,0.362478,-3.5587
86,4.845938\C,0,0.428027,-2.154778,3.17601\C,0,-0.078816,-0.926491,2.6
8633\H,0,0.274329,-0.519187,1.736303\C,0,-1.006796,-0.200796,3.429945\
H,0,-1.371773,0.752816,3.037219\C,0,1.403641,-2.937189,2.402355\C,0,2.
426712,-3.767474,3.117788\H,0,3.325139,-3.915549,2.498661\H,0,2.01044,
-4.762785,3.3587\H,0,2.704368,-3.280514,4.064871\N,0,1.372655,-2.85735
2,1.090101\H,0,0.606212,-2.27416,0.599507\C,0,2.20945,-3.520338,0.1374
94\C,0,2.717731,-2.750206,-0.925311\H,0,2.5404,-1.672167,-0.960912\C,0
,3.477148,-3.373817,-1.922648\H,0,3.87709,-2.770691,-2.742866\C,0,3.73
0136,-4.753178,-1.864869\C,0,3.213604,-5.515541,-0.805085\H,0,3.39546,
-6.594493,-0.761647\C,0,2.444424,-4.907006,0.195838\H,0,2.004112,-5.50
8078,0.99558\C,0,3.48478,1.206269,-0.711889\C,0,4.057083,0.722082,-1.9
16024\C,0,3.96308,0.739105,0.545938\C,0,5.115808,-0.204856,-1.837164\C
,0,5.014713,-0.191689,0.569146\C,0,5.604654,-0.681054,-0.610959\H,0,5.
5625,-0.584316,-2.763753\H,0,5.383773,-0.549263,1.535242\C,0,-3.980424
,-0.362854,-0.592434\C,0,-4.216442,-1.600085,0.066686\C,0,-4.420837,-0
.179444,-1.933762\C,0,-4.908221,-2.615482,-0.622588\C,0,-5.101691,-1.2
26538,-2.577836\C,0,-5.361243,-2.453411,-1.94095\H,0,-5.093554,-3.5707
58,-0.11618\H,0,-5.446515,-1.075668,-3.607584\H,0,4.325067,-5.234896,-

2.647885\C,0,-2.523635,0.111107,5.433506\H,0,-3.465263,0.161198,4.8551
97\H,0,-2.742457,-0.343867,6.413387\H,0,-2.192947,1.153222,5.592985\C,
0,-4.211482,1.135438,-2.687878\H,0,-3.636375,1.814774,-2.037095\C,0,-3
.720329,-1.878277,1.487151\C,0,-6.116791,-3.571614,-2.654339\H,0,-6.14
501,-4.434986,-1.963017\C,0,-4.88892,-1.972418,2.489305\H,0,-4.50968,-
2.149673,3.512606\H,0,-5.485721,-1.042881,2.50159\H,0,-5.568433,-2.806
711,2.233482\C,0,-5.395604,-4.024369,-3.940333\H,0,-5.354973,-3.208632
,-4.685447\H,0,-4.358973,-4.340993,-3.727378\H,0,-5.926608,-4.875625,-
4.404737\C,0,-7.574175,-3.161769,-2.952167\H,0,-8.129002,-3.99836,-3.4
15566\H,0,-8.103784,-2.868803,-2.027948\H,0,-7.611361,-2.305058,-3.650
321\C,0,-3.389343,0.933473,-3.976782\H,0,-3.927569,0.299655,-4.705724\
H,0,-3.192509,1.907261,-4.462227\H,0,-2.41928,0.459801,-3.750816\C,0,-
5.559098,1.82818,-2.97985\H,0,-5.395071,2.802725,-3.475716\H,0,-6.1932
68,1.213746,-3.645309\H,0,-6.122913,2.009802,-2.046998\C,0,6.749983,-1
.689999,-0.5687\H,0,6.839995,-2.115217,-1.586294\C,0,3.558595,1.188375
,-3.285056\H,0,2.586931,1.687553,-3.127134\C,0,3.381855,1.277237,1.856
181\H,0,2.315401,1.499256,1.678472\C,0,8.085058,-0.989475,-0.236153\H,
0,8.921627,-1.712275,-0.250661\H,0,8.308839,-0.189779,-0.964591\H,0,8.
047304,-0.531347,0.769749\C,0,6.482404,-2.855178,0.404198\H,0,6.455676
,-2.509525,1.453758\H,0,5.520417,-3.349461,0.182615\H,0,7.283275,-3.61
2873,0.327505\C,0,3.443148,0.272343,3.019914\H,0,3.039284,-0.710206,2.
723786\H,0,4.476195,0.121119,3.382673\H,0,2.84605,0.644106,3.871358\C,
0,4.068608,2.604094,2.247969\H,0,3.976026,3.357404,1.446343\H,0,3.6144
45,3.02218,3.165276\H,0,5.145191,2.441447,2.440588\C,0,4.530792,2.2195
51,-3.896614\H,0,4.668989,3.089544,-3.230829\H,0,5.524911,1.767212,-4.
071603\H,0,4.149514,2.588176,-4.866831\C,0,3.306982,0.018743,-4.255803
\H,0,2.887194,0.40279,-5.203896\H,0,4.238658,-0.521907,-4.504231\H,0,2
.578078,-0.686219,-3.824415\C,0,-2.83138,-3.136987,1.547764\H,0,-3.405
939,-4.055154,1.324938\H,0,-2.002695,-3.053794,0.825605\H,0,-2.40214,-
3.249396,2.560089\H,0,-3.08899,-1.028144,1.791982\\Version=ES64L-G09Re
vD.01\State=1-A\HF=-3216.0973304\RMSD=6.007e-09\Dipole=1.708134,-2.421
8302,5.0102926\Quadrupole=-8.2872772,12.7295441,-4.442267,-17.3134219,
-4.928402,-13.6000131\PG=C01 [X(C65H72N1O4P1)]\\@

Conf1

1\1\GINC-WORKER2\SP\RTPSSTPSS\def2SVP\C65H72N1O4P1\JHIOE\05-May-2019\0
\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(smd,
solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,-0.101
954,-0.381699,-1.301615\O,0,-1.385719,0.68041,-1.476842\O,0,0.823327,0
.492836,-0.17659\O,0,0.554728,-0.465515,-2.647403\O,0,-0.517626,-1.600
693,-0.484293\C,0,-1.263055,2.340934,0.242693\C,0,-1.95202,1.296689,-0
.381248\C,0,-3.266946,0.885425,0.004014\C,0,-3.867256,1.546746,1.06707
5\H,0,-4.883068,1.270843,1.3685\C,0,-3.184311,2.554967,1.805894\C,0,-1
.852605,2.946971,1.412144\C,0,-1.156077,3.883852,2.234627\H,0,-0.1288,
4.158197,1.979161\C,0,-1.753245,4.432632,3.360238\H,0,-1.192982,5.1414
83,3.979868\C,0,-3.08106,4.078039,3.720394\H,0,-3.543724,4.5236,4.6077
56\C,0,-3.777705,3.153619,2.958148\H,0,-4.793118,2.851335,3.238783\C,0
,0.070069,2.767785,-0.272017\C,0,1.094351,1.825007,-0.40823\C,0,2.4504
14,2.182934,-0.686861\C,0,2.732089,3.518056,-0.940661\H,0,3.764549,3.8
23737,-1.139445\C,0,1.706396,4.5076,-0.962639\C,0,0.353436,4.136701,-0
.626142\C,0,-0.659297,5.14074,-0.693906\H,0,-1.695854,4.867359,-0.4757
06\C,0,-0.350395,6.445938,-1.048306\H,0,-1.14661,7.196585,-1.102914\C,
0,0.987973,6.816013,-1.348551\H,0,1.219782,7.851278,-1.621702\C,0,1.99
321,5.862532,-1.308233\H,0,3.027119,6.13154,-1.553061\C,0,-1.57454,-0.
652599,4.584802\C,0,-1.107824,-1.897052,5.058124\H,0,-1.49024,-2.29172
2,6.005855\C,0,-0.163586,-2.637863,4.339718\H,0,0.172505,-3.601691,4.7
33764\C,0,0.31245,-2.170405,3.09205\C,0,-0.143056,-0.916083,2.618567\H
,0,0.23953,-0.50428,1.681967\C,0,-1.058425,-0.172837,3.360745\H,0,-1.3
84547,0.799991,2.98052\C,0,1.268749,-2.975212,2.317035\C,0,2.254938,-3
.850896,3.030236\H,0,3.158867,-4.010372,2.421629\H,0,1.80621,-4.839041
,3.240344\H,0,2.53092,-3.395106,3.993061\N,0,1.251656,-2.879156,1.0055
95\H,0,0.510859,-2.262893,0.515859\C,0,2.072056,-3.56132,0.052336\C,0,
2.612456,-2.799783,-1.000854\H,0,2.471471,-1.716263,-1.028694\C,0,3.35
6902,-3.439834,-1.9989\H,0,3.783034,-2.843566,-2.810815\C,0,3.56236,-4
.827556,-1.95245\C,0,3.014219,-5.581007,-0.902325\H,0,3.159199,-6.6658
13,-0.867211\C,0,2.260829,-4.95535,0.10005\H,0,1.79691,-5.548425,0.892
258\C,0,3.524456,1.138065,-0.62299\C,0,4.112799,0.627485,-1.808033\C,0
,3.952326,0.663004,0.650547\C,0,5.138819,-0.333097,-1.695663\C,0,4.972
217,-0.300692,0.706965\C,0,5.579985,-0.814652,-0.453896\H,0,5.599313,-
0.73152,-2.607321\H,0,5.30627,-0.663537,1.684094\C,0,-3.966786,-0.2152
41,-0.733828\C,0,-4.210479,-1.461862,-0.091261\C,0,-4.404503,-0.010114
,-2.070005\C,0,-4.916526,-2.458668,-0.787945\C,0,-5.100324,-1.043492,-
2.725746\C,0,-5.37396,-2.272556,-2.10443\H,0,-5.105201,-3.416059,-0.28
8621\H,0,-5.445259,-0.884575,-3.754983\H,0,4.145345,-5.322255,-2.73634
\C,0,-2.5983,0.152558,5.344667\H,0,-3.501252,0.309655,4.726329\H,0,-2.
898147,-0.346618,6.280574\H,0,-2.20446,1.155391,5.591544\C,0,-4.169002
,1.308093,-2.809557\H,0,-3.594201,1.973064,-2.143499\C,0,-3.707342,-1.

758119,1.322827\C,0,-6.133401,-3.373288,-2.840045\H,0,-6.381927,-2.981
24,-3.8444\C,0,-4.859849,-1.762402,2.347931\H,0,-4.472203,-1.947593,3.
366632\H,0,-5.398337,-0.798457,2.356639\H,0,-5.593484,-2.556844,2.1154
88\C,0,-7.459068,-3.71985,-2.131308\H,0,-7.276344,-4.135655,-1.12312\H
,0,-8.097893,-2.82561,-2.018345\H,0,-8.024631,-4.474811,-2.707971\C,0,
-5.261677,-4.631745,-3.030385\H,0,-5.803828,-5.397618,-3.615088\H,0,-4
.32467,-4.391611,-3.563809\H,0,-4.991463,-5.079924,-2.05642\C,0,-3.329
358,1.104892,-4.087181\H,0,-3.865235,0.485093,-4.829706\H,0,-3.110288,
2.079674,-4.561024\H,0,-2.370144,0.614757,-3.849938\C,0,-5.50193,2.022
158,-3.115874\H,0,-5.316897,2.998744,-3.600143\H,0,-6.134353,1.423003,
-3.796673\H,0,-6.077263,2.203131,-2.189931\C,0,6.686791,-1.862333,-0.3
65121\H,0,6.88289,-2.212807,-1.396109\C,0,3.668749,1.106805,-3.191069\
H,0,2.702524,1.624359,-3.061616\C,0,3.352047,1.226652,1.941528\H,0,2.2
96412,1.474268,1.734008\C,0,7.993801,-1.246114,0.177301\H,0,8.805109,-
1.997112,0.188151\H,0,8.32253,-0.394141,-0.444301\H,0,7.857508,-0.8787
8,1.211528\C,0,6.264536,-3.086687,0.472739\H,0,6.088739,-2.812435,1.52
9212\H,0,5.337707,-3.538293,0.078956\H,0,7.056192,-3.857928,0.456882\C
,0,3.358395,0.231043,3.114917\H,0,2.938889,-0.744647,2.818041\H,0,4.37
7691,0.059514,3.506446\H,0,2.748106,0.624954,3.94682\C,0,4.063015,2.53
8174,2.342035\H,0,4.008571,3.289191,1.535021\H,0,3.598574,2.972964,3.2
46334\H,0,5.130209,2.348881,2.560646\C,0,4.681318,2.119497,-3.766704\H
,0,4.820002,2.981882,-3.091351\H,0,5.669515,1.645399,-3.91578\H,0,4.33
6425,2.502307,-4.74499\C,0,3.424265,-0.052506,-4.175599\H,0,3.04511,0.
345224,-5.135089\H,0,4.351318,-0.61281,-4.396028\H,0,2.665418,-0.74233
3,-3.772737\C,0,-2.906032,-3.073623,1.389567\H,0,-3.546387,-3.955091,1
.200856\H,0,-2.090188,-3.062133,0.64872\H,0,-2.462694,-3.194868,2.3946
7\H,0,-3.014469,-0.948273,1.602377\\Version=ES64L-G09RevD.01\State=1-A
\HF=-3216.0974305\RMSD=6.114e-09\Dipole=1.5336404,-2.5800941,5.0002904
\Quadrupole=-9.3084686,14.6792822,-5.3708136,-16.250315,-5.5550033,-12
.5917013\PG=C01 [X(C65H72N1O4P1)]\\@

Conf2

1\1\GINC-WORKER0\SP\RTPSSTPSS\def2SVP\C65H72N1O4P1\JHIOE\06-May-2019\0
\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(smd,
solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,-0.065
194,-0.472512,-1.22955\O,0,-1.286101,0.637643,-1.51914\O,0,0.849498,0.
412355,-0.101712\O,0,0.64751,-0.656324,-2.535968\O,0,-0.584102,-1.6221
75,-0.371724\C,0,-1.205624,2.333403,0.164606\C,0,-1.893667,1.296917,-0
.471989\C,0,-3.240456,0.936478,-0.151613\C,0,-3.878041,1.646853,0.8565
22\H,0,-4.918442,1.414009,1.105324\C,0,-3.205642,2.655461,1.604662\C,0
,-1.840855,2.992651,1.279752\C,0,-1.161246,3.929772,2.115875\H,0,-0.11
1806,4.161719,1.913904\C,0,-1.804039,4.531229,3.188242\H,0,-1.25691,5.
239152,3.820539\C,0,-3.162217,4.231455,3.478097\H,0,-3.66028,4.717706,
4.323881\C,0,-3.844441,3.307768,2.701975\H,0,-4.88396,3.046624,2.93058
5\C,0,0.164754,2.705571,-0.291004\C,0,1.166606,1.729947,-0.357648\C,0,
2.541686,2.044705,-0.587207\C,0,2.871435,3.366844,-0.854868\H,0,3.9202
32,3.638935,-1.012725\C,0,1.8778,4.383402,-0.947264\C,0,0.50142,4.0566
38,-0.666922\C,0,-0.478423,5.085616,-0.809599\H,0,-1.531745,4.846673,-
0.637623\C,0,-0.116648,6.372473,-1.180468\H,0,-0.888677,7.141732,-1.29
2788\C,0,1.244363,6.699645,-1.42358\H,0,1.517731,7.720958,-1.7104\C,0,
2.219124,5.720826,-1.311437\H,0,3.270787,5.954763,-1.512885\C,0,-1.921
889,-0.360087,4.605463\C,0,-1.576178,-1.614399,5.151615\H,0,-2.04697,-
1.945026,6.083993\C,0,-0.641997,-2.444282,4.523918\H,0,-0.400224,-3.41
3352,4.970665\C,0,-0.050615,-2.056622,3.298533\C,0,-0.383713,-0.793036
,2.752458\H,0,0.0875,-0.44484,1.829588\C,0,-1.29206,0.037678,3.405505\
H,0,-1.52323,1.015058,2.972407\C,0,0.901489,-2.948165,2.620381\C,0,1.7
60375,-3.874738,3.42588\H,0,2.67556,-4.150214,2.880136\H,0,1.204104,-4
.80331,3.651043\H,0,2.024746,-3.401339,4.383722\N,0,0.994682,-2.882512
,1.311177\H,0,0.324887,-2.248724,0.745266\C,0,1.855139,-3.621699,0.439
035\C,0,2.551866,-2.894836,-0.544812\H,0,2.49388,-1.803106,-0.56625\C,
0,3.336754,-3.582766,-1.477343\H,0,3.881387,-3.015547,-2.237515\C,0,3.
428466,-4.983176,-1.431963\C,0,2.726524,-5.700108,-0.450337\H,0,2.7839
87,-6.793202,-0.418634\C,0,1.929975,-5.025612,0.485561\H,0,1.348163,-5
.58391,1.22388\C,0,3.608613,0.996298,-0.467499\C,0,4.261855,0.496822,-
1.625299\C,0,4.009699,0.554009,0.823726\C,0,5.356848,-0.374327,-1.4658
18\C,0,5.107279,-0.319659,0.928888\C,0,5.813982,-0.773933,-0.198342\H,
0,5.8714,-0.743255,-2.360479\H,0,5.44029,-0.6468,1.92042\C,0,-3.933185
,-0.156989,-0.907011\C,0,-4.239758,-1.388636,-0.262772\C,0,-4.298089,0
.042403,-2.265475\C,0,-4.935155,-2.376646,-0.982545\C,0,-4.984536,-0.9
8249,-2.944037\C,0,-5.319229,-2.196498,-2.323207\H,0,-5.174107,-3.3224
21,-0.48274\H,0,-5.27192,-0.82947,-3.991676\H,0,4.044648,-5.515525,-2.
164138\C,0,-2.943499,0.534367,5.261085\H,0,-3.83936,0.626133,4.618619\
H,0,-3.260319,0.142854,6.241627\H,0,-2.545488,1.555599,5.39786\C,0,-3.
991988,1.344923,-3.007032\H,0,-3.435169,2.003831,-2.319846\C,0,-3.8191
9,-1.674398,1.180342\C,0,-6.062029,-3.28908,-3.087411\H,0,-6.250925,-2
.900513,-4.105952\C,0,-5.019746,-1.589226,2.145714\H,0,-4.695944,-1.77

0254,3.187218\H,0,-5.504283,-0.598068,2.104829\H,0,-5.783543,-2.34802,
1.892152\C,0,-7.42873,-3.607695,-2.447125\H,0,-7.306769,-4.023614,-1.4
29838\H,0,-8.05612,-2.701652,-2.369994\H,0,-7.977034,-4.353934,-3.0511
31\C,0,-5.204544,-4.564409,-3.224402\H,0,-5.727833,-5.322842,-3.835425
\H,0,-4.23493,-4.344246,-3.705733\H,0,-4.997827,-5.012938,-2.235116\C,
0,-3.093255,1.104761,-4.237228\H,0,-3.605615,0.488957,-4.999355\H,0,-2
.82519,2.067535,-4.710406\H,0,-2.160253,0.594503,-3.944517\C,0,-5.2897
81,2.086871,-3.388688\H,0,-5.056873,3.052718,-3.873738\H,0,-5.901101,1
.494229,-4.093986\H,0,-5.906618,2.292568,-2.495118\C,0,7.041335,-1.668
246,-0.036983\H,0,7.234058,-1.75515,1.049069\C,0,3.814415,0.898727,-3.
032118\H,0,2.830559,1.389221,-2.935002\C,0,3.306341,1.061221,2.08535\H
,0,2.261591,1.28576,1.810874\C,0,6.796689,-3.090636,-0.579221\H,0,7.68
6189,-3.726673,-0.415904\H,0,5.937788,-3.566892,-0.075904\H,0,6.588922
,-3.073458,-1.66478\C,0,8.290385,-1.035431,-0.683541\H,0,8.174781,-0.9
51765,-1.779765\H,0,8.478202,-0.022687,-0.28394\H,0,9.185737,-1.653413
,-0.487299\C,0,3.257473,0.020442,3.218168\H,0,2.879269,-0.950454,2.854
858\H,0,4.252618,-0.148022,3.668367\H,0,2.586867,0.3696,4.023263\C,0,3
.944829,2.377967,2.577633\H,0,3.921031,3.151992,1.790715\H,0,3.402426,
2.768073,3.458622\H,0,4.999877,2.216261,2.866273\C,0,4.79577,1.912476,
-3.656813\H,0,4.901606,2.813288,-3.027145\H,0,5.800162,1.465412,-3.778
703\H,0,4.443054,2.232752,-4.654588\C,0,3.616055,-0.321392,-3.9526\H,0
,3.238195,0.008207,-4.937984\H,0,4.563033,-0.864439,-4.12729\H,0,2.873
659,-1.011813,-3.520984\C,0,-3.098062,-3.029848,1.322043\H,0,-3.776786
,-3.879828,1.123778\H,0,-2.245072,-3.086189,0.626422\H,0,-2.715084,-3.
14706,2.351861\H,0,-3.096704,-0.894935,1.472031\\Version=ES64L-G09RevD
.01\State=1-A\HF=-3216.0960396\RMSD=2.058e-09\Dipole=1.0498946,-2.3514
819,5.2624789\Quadrupole=-9.5013742,13.4643226,-3.9629484,-13.5367305,
-6.4079337,-15.0884697\PG=C01 [X(C65H72N1O4P1)]\\@

Conf3

1\1\GINC-WORKER2\SP\RTPSSTPSS\def2SVP\C65H72N1O4P1\JHIOE\06-May-2019\0
\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(smd,
solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,-0.090
393,-0.541341,-1.174492\O,0,-1.350103,0.526771,-1.454139\O,0,0.836758,
0.400252,-0.103878\O,0,0.584213,-0.744615,-2.498014\O,0,-0.548967,-1.6
78426,-0.266704\C,0,-1.263845,2.268832,0.181636\C,0,-1.942186,1.19706,
-0.404913\C,0,-3.267009,0.808618,-0.031728\C,0,-3.891736,1.528175,0.97
8073\H,0,-4.917402,1.274986,1.265318\C,0,-3.223964,2.573342,1.678608\C
,0,-1.880435,2.939244,1.300527\C,0,-1.201052,3.916347,2.089683\H,0,-0.
165787,4.172117,1.847347\C,0,-1.825543,4.52711,3.167591\H,0,-1.278623,
5.266249,3.76327\C,0,-3.164424,4.19731,3.509972\H,0,-3.648308,4.690872
,4.359759\C,0,-3.844972,3.235422,2.780192\H,0,-4.868532,2.951338,3.049
776\C,0,0.078615,2.667111,-0.330283\C,0,1.105922,1.719156,-0.405246\C,
0,2.462225,2.067911,-0.689656\C,0,2.743837,3.391516,-1.001459\H,0,3.77
8809,3.688438,-1.200747\C,0,1.718256,4.376559,-1.085267\C,0,0.36228,4.
017047,-0.750645\C,0,-0.652987,5.012094,-0.886043\H,0,-1.692441,4.7449
43,-0.674527\C,0,-0.342615,6.299489,-1.299041\H,0,-1.140629,7.042724,-
1.404642\C,0,0.999586,6.66072,-1.593823\H,0,1.23242,7.682644,-1.912531
\C,0,2.006985,5.714345,-1.491409\H,0,3.043903,5.974773,-1.732839\C,0,-
1.762359,-0.333249,4.717655\C,0,-1.343062,-1.555447,5.284581\H,0,-1.76
5546,-1.879488,6.24214\C,0,-0.395245,-2.361632,4.646254\H,0,-0.095295,
-3.306132,5.109864\C,0,0.135683,-1.983554,3.390664\C,0,-0.272199,-0.75
2068,2.82254\H,0,0.151361,-0.410648,1.874398\C,0,-1.19352,0.056438,3.4
85071\H,0,-1.48287,1.010085,3.034723\C,0,1.101822,-2.852306,2.702727\C
,0,2.031586,-3.714957,3.501162\H,0,2.937013,-3.967451,2.928421\H,0,1.5
26347,-4.659247,3.775681\H,0,2.310341,-3.200263,4.433238\N,0,1.14428,-
2.821242,1.389902\H,0,0.426483,-2.234905,0.831551\C,0,2.00202,-3.55293
6,0.508707\C,0,2.642569,-2.830492,-0.515509\H,0,2.548722,-1.741904,-0.
563241\C,0,3.417927,-3.518772,-1.45581\H,0,3.919458,-2.955712,-2.24782
3\C,0,3.55614,-4.913839,-1.377821\C,0,2.910595,-5.626188,-0.355068\H,0
,3.004738,-6.715642,-0.297006\C,0,2.123765,-4.951909,0.589082\H,0,1.58
4898,-5.507435,1.361319\C,0,3.563628,1.055417,-0.578293\C,0,4.191929,0
.542321,-1.743659\C,0,4.018945,0.660739,0.710352\C,0,5.316326,-0.29324
4,-1.597693\C,0,5.144645,-0.177808,0.802031\C,0,5.826595,-0.643574,-0.
33592\H,0,5.811885,-0.671926,-2.499058\H,0,5.519143,-0.467672,1.790306
\C,0,-3.954991,-0.322138,-0.734553\C,0,-4.21732,-1.538027,-0.046037\C,
0,-4.36713,-0.169834,-2.087684\C,0,-4.924413,-2.55639,-0.714403\C,0,-5
.060202,-1.221271,-2.712287\C,0,-5.359786,-2.420721,-2.042182\H,0,-5.1
36368,-3.49367,-0.185753\H,0,-5.381105,-1.095826,-3.753114\H,0,4.16505
1,-5.445613,-2.11647\C,0,-2.797231,0.536664,5.385513\H,0,-3.722285,0.5
64081,4.779294\H,0,-3.055091,0.166539,6.391319\H,0,-2.442137,1.579078,
5.470161\C,0,-4.104441,1.112656,-2.879673\H,0,-3.533579,1.801353,-2.23
4774\C,0,-3.737665,-1.77886,1.386639\C,0,-6.116747,-3.548967,-2.737656
\H,0,-6.264066,-4.349022,-1.987874\C,0,-4.901059,-1.697252,2.396646\H,
0,-4.531413,-1.847277,3.427728\H,0,-5.407726,-0.717364,2.35355\H,0,-5.
657863,-2.477592,2.192205\C,0,-5.29617,-4.144183,-3.900844\H,0,-5.1266

4,-3.392854,-4.694167\H,0,-4.309163,-4.497647,-3.552858\H,0,-5.827996,
-5.000431,-4.355336\C,0,-7.510107,-3.094349,-3.218123\H,0,-8.065225,-3
.941874,-3.660553\H,0,-8.109496,-2.690614,-2.382487\H,0,-7.430836,-2.3
06896,-3.990304\C,0,-3.244823,0.841921,-4.131346\H,0,-3.772722,0.18988
8,-4.851645\H,0,-3.00992,1.790372,-4.64894\H,0,-2.293696,0.35761,-3.85
3145\C,0,-5.424222,1.8252,-3.241049\H,0,-5.220923,2.778282,-3.763266\H
,0,-6.049952,1.20279,-3.907052\H,0,-6.014662,2.050806,-2.334535\C,0,7.
0867,-1.494518,-0.191278\H,0,7.31354,-1.549551,0.890279\C,0,3.686265,0
.893402,-3.144462\H,0,2.695478,1.364794,-3.026066\C,0,3.33999,1.183056
,1.979426\H,0,2.27892,1.359501,1.733968\C,0,6.874788,-2.936232,-0.6945
56\H,0,7.789489,-3.538451,-0.542773\H,0,6.046509,-3.428887,-0.157116\H
,0,6.636819,-2.950855,-1.773916\C,0,8.295183,-0.836922,-0.888572\H,0,8
.144643,-0.782521,-1.98241\H,0,8.461818,0.19017,-0.51715\H,0,9.215266,
-1.421862,-0.705879\C,0,3.3668,0.180294,3.146894\H,0,3.004676,-0.81319
1,2.831554\H,0,4.38287,0.05646,3.563701\H,0,2.716708,0.5373,3.965261\C
,0,3.942962,2.53816,2.408664\H,0,3.866591,3.284781,1.598929\H,0,3.4125
66,2.936519,3.293234\H,0,5.011556,2.42547,2.669511\C,0,4.620256,1.9105
94,-3.83253\H,0,4.728251,2.830525,-3.231306\H,0,5.629587,1.482889,-3.9
80399\H,0,4.223281,2.195326,-4.824435\C,0,3.483026,-0.356833,-4.0224\H
,0,3.068507,-0.063449,-5.004492\H,0,4.434445,-0.887215,-4.211203\H,0,2
.767559,-1.046755,-3.547146\C,0,-2.978977,-3.113494,1.530161\H,0,-3.64
377,-3.98331,1.375537\H,0,-2.151644,-3.164486,0.803847\H,0,-2.554883,-
3.198084,2.54712\H,0,-3.022821,-0.976835,1.631844\\Version=ES64L-G09Re
vD.01\State=1-A\HF=-3216.0960294\RMSD=2.052e-09\Dipole=1.3180727,-2.12
30292,5.2663943\Quadrupole=-8.9319945,11.2411187,-2.3091242,-14.992139
8,-5.0747244,-15.696795\PG=C01 [X(C65H72N1O4P1)]\\@

TRIP/1E Type III.1

1\1\GINC-WORKER1\SP\RTPSSTPSS\def2SVP\C65H72N1O4P1\JHIOE\27-Mar-2019\0
\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(smd,
solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\H,0,-5.712
31,0.551506,-2.0845\C,0,-5.217347,0.454445,-1.110205\C,0,-4.140798,1.3
05227,-0.80799\C,0,-5.703145,-0.49898,-0.195541\C,0,-3.503063,1.185282
,0.457582\C,0,-3.725315,2.370052,-1.825077\C,0,-5.030883,-0.626222,1.0
29857\C,0,-6.953155,-1.306385,-0.545022\C,0,-2.42593,2.147774,0.85695\
C,0,-3.930427,0.184386,1.371492\C,0,-4.860968,3.387137,-2.062421\C,0,-
3.243194,1.746094,-3.149402\H,0,-2.875635,2.930265,-1.400273\H,0,-5.17
4929,3.86192,-1.115281\H,0,-5.748612,2.903864,-2.510859\H,0,-4.528172,
4.185379,-2.751306\H,0,-2.89849,2.536293,-3.841821\H,0,-4.055396,1.190
618,-3.653172\H,0,-2.402716,1.055504,-2.970615\H,0,-5.366268,-1.37636,
1.75267\C,0,-8.201823,-0.395391,-0.504575\C,0,-7.168786,-2.549115,0.33
2149\H,0,-6.827527,-1.64689,-1.590917\H,0,-8.090667,0.471759,-1.179232
\H,0,-8.368168,-0.01002,0.518567\H,0,-9.105163,-0.954128,-0.811629\H,0
,-7.416856,-2.272411,1.373458\H,0,-6.273674,-3.194138,0.356186\H,0,-8.
010507,-3.147846,-0.05939\C,0,-1.137088,2.130885,0.237809\C,0,-2.65269
4,3.093675,1.849275\C,0,-3.242342,-0.042412,2.720695\O,0,-0.927382,1.2
4762,-0.802506\C,0,-0.10798,3.008405,0.59368\H,0,-3.640855,3.153937,2.
316966\C,0,-1.626806,3.968707,2.306727\C,0,-2.83326,-1.515782,2.922745
\C,0,-4.124488,0.444851,3.889406\H,0,-2.313553,0.552578,2.725203\H,0,-
2.270968,-1.626423,3.86844\H,0,-2.185669,-1.849489,2.097376\H,0,-3.712
786,-2.183394,2.979935\H,0,-3.600558,0.312914,4.854166\H,0,-4.383492,1
.513091,3.785832\H,0,-5.069366,-0.128315,3.936357\P,0,0.024963,-0.1127
46,-0.558885\C,0,1.18566,2.95481,-0.143659\C,0,-0.321382,3.912207,1.69
657\C,0,-1.859456,4.882297,3.379062\O,0,-0.637989,-1.043995,0.45019\O,
0,0.442926,-0.593453,-1.923892\O,0,1.291191,0.597333,0.290182\C,0,1.86
9025,1.737737,-0.238549\C,0,1.766758,4.119052,-0.764902\C,0,0.711303,4
.737011,2.23804\H,0,-2.860187,4.920213,3.824412\C,0,-0.841782,5.690978
,3.859415\C,0,3.183948,1.626376,-0.78989\C,0,1.076792,5.365092,-0.8697
3\C,0,3.087997,4.021611,-1.334318\H,0,1.719887,4.67292,1.820215\C,0,0.
457467,5.603986,3.290717\H,0,-1.030564,6.384838,4.685912\C,0,3.775632,
2.774443,-1.29904\C,0,3.917514,0.319321,-0.751717\H,0,0.057407,5.44422
,-0.480791\C,0,1.673064,6.465077,-1.468648\C,0,3.679461,5.176415,-1.93
01\H,0,1.268285,6.22248,3.691318\H,0,4.795324,2.724908,-1.694251\C,0,4
.463858,-0.134912,0.479888\C,0,4.097262,-0.443371,-1.936127\H,0,1.1205
83,7.408177,-1.544071\C,0,2.99088,6.377503,-1.992591\H,0,4.688617,5.08
904,-2.348807\C,0,5.19731,-1.335516,0.499726\C,0,4.307139,0.670098,1.7
72286\C,0,4.852842,-1.629645,-1.865876\C,0,3.507492,0.000032,-3.276822
\H,0,3.453025,7.255511,-2.456998\H,0,5.62096,-1.679258,1.450826\C,0,5.
41594,-2.093282,-0.665503\C,0,5.6759,1.131322,2.31387\C,0,3.508777,-0.
099487,2.842554\H,0,3.732543,1.580887,1.53345\H,0,5.54296,1.762643,3.2
11557\H,0,6.224673,1.721477,1.5579\H,0,6.309492,0.270971,2.598242\H,0,
3.361238,0.532416,3.737787\H,0,4.039556,-1.014128,3.163075\H,0,2.51655
1,-0.388831,2.458192\H,0,5.01102,-2.217028,-2.778191\C,0,4.580317,0.66
8824,-4.162686\C,0,2.825261,-1.15497,-4.035107\H,0,2.72548,0.746581,-3
.056585\H,0,4.137943,1.013369,-5.115793\H,0,5.037698,1.541057,-3.66456
7\H,0,5.390151,-0.045491,-4.40261\H,0,2.309686,-0.761962,-4.9307\H,0,2
.072663,-1.643925,-3.396469\H,0,3.555145,-1.909563,-4.381889\C,0,6.232

864,-3.383248,-0.642177\C,0,7.643648,-3.163895,-0.059771\C,0,5.494758,
-4.511189,0.107631\H,0,6.350503,-3.704853,-1.69421\H,0,7.598879,-2.879
524,1.007736\H,0,8.18077,-2.365061,-0.601885\H,0,8.241614,-4.090645,-0
.133315\H,0,5.35467,-4.2542,1.172832\H,0,6.073209,-5.452389,0.060903\H
,0,4.498449,-4.698239,-0.32989\H,0,-5.368708,-2.688743,-3.968513\C,0,-
4.574688,-2.844753,-3.230768\C,0,-3.364051,-2.142045,-3.33877\C,0,-4.7
73963,-3.732776,-2.162535\H,0,-3.207999,-1.435232,-4.159728\C,0,-2.345
334,-2.336144,-2.397979\H,0,-5.727193,-4.26002,-2.055216\C,0,-3.766704
,-3.934937,-1.209398\H,0,-1.394618,-1.795554,-2.473675\C,0,-2.543217,-
3.252589,-1.346806\H,0,-3.944203,-4.591086,-0.354196\N,0,-1.468529,-3.
408828,-0.416791\C,0,-0.98909,-4.517979,0.101815\H,0,-1.04031,-2.46484
8,-0.095288\C,0,-1.566988,-5.867845,-0.198602\C,0,0.178772,-4.416968,0
.991379\H,0,-2.324491,-6.132302,0.562205\H,0,-2.058468,-5.886202,-1.18
386\H,0,-0.773756,-6.629507,-0.163137\C,0,0.299726,-5.29013,2.099502\C
,0,1.206082,-3.475074,0.750955\H,0,-0.477895,-6.033995,2.298488\C,0,1.
387444,-5.181516,2.967819\H,0,1.171075,-2.834609,-0.133895\C,0,2.30350
2,-3.397637,1.610735\H,0,1.450188,-5.847668,3.835617\C,0,2.407197,-4.2
29581,2.745069\H,0,3.098599,-2.680581,1.389268\C,0,3.565382,-4.10036,3
.703011\H,0,3.91352,-5.088827,4.050079\H,0,3.255882,-3.530575,4.600165
\H,0,4.412804,-3.565968,3.244565\\Version=ES64L-G09RevD.01\State=1-A\H
F=-3216.0898631\RMSD=5.297e-09\Dipole=-1.2847597,-4.7048372,1.2564765\
Quadrupole=-5.0187217,26.9891532,-21.9704314,14.9074858,11.1982848,-7.
1062127\PG=C01 [X(C65H72N1O4P1)]\\@

TRIP/1E Type III.2

1\1\GINC-WORKER2\SP\RTPSSTPSS\def2SVP\C65H72N1O4P1\JHIOE\27-Mar-2019\0
\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(smd,
solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,0.1771
26,-0.15514,-0.393091\O,0,-0.60123,1.287684,-0.753639\O,0,1.508061,0.4
672,0.424385\O,0,0.540274,-0.785479,-1.710831\O,0,-0.597575,-0.909954,
0.68035\C,0,0.412979,3.042288,0.519768\C,0,-0.709295,2.264679,0.215221
\C,0,-1.992989,2.476696,0.808751\C,0,-2.120315,3.519287,1.717083\H,0,-
3.1006,3.736591,2.153462\C,0,-1.004065,4.307122,2.120215\C,0,0.292832,
4.051997,1.542681\C,0,1.407269,4.797432,2.035136\H,0,2.406299,4.584585
,1.644291\C,0,1.24312,5.774,3.006635\H,0,2.115023,6.328554,3.370867\C,
0,-0.043506,6.056097,3.53898\H,0,-0.160304,6.834836,4.300557\C,0,-1.14
1657,5.329168,3.107756\H,0,-2.135958,5.518492,3.528317\C,0,1.699663,2.
777864,-0.185401\C,0,2.226499,1.482036,-0.177438\C,0,3.519449,1.159949
,-0.696914\C,0,4.257224,2.181195,-1.279331\H,0,5.263705,1.973373,-1.65
6693\C,0,3.732498,3.498837,-1.41974\C,0,2.429167,3.807377,-0.883509\C,
0,1.904896,5.118114,-1.097955\H,0,0.901657,5.357225,-0.733689\C,0,2.64
0261,6.08286,-1.770959\H,0,2.212132,7.078962,-1.928479\C,0,3.939626,5.
788068,-2.2639\H,0,4.512868,6.560453,-2.788245\C,0,4.469368,4.518622,-
2.094425\H,0,5.462111,4.27148,-2.487562\C,0,4.052042,-0.234865,-0.5597
01\C,0,4.141199,-1.089865,-1.69361\C,0,4.468258,-0.699937,0.716127\C,0
,4.662515,-2.385349,-1.525379\C,0,4.986744,-2.003875,0.829936\C,0,5.09
3903,-2.863767,-0.274878\H,0,4.734731,-3.042906,-2.39901\H,0,5.318625,
-2.362151,1.812139\C,0,-3.164795,1.614547,0.444378\C,0,-3.674233,0.672
06,1.377699\C,0,-3.790636,1.765123,-0.823223\C,0,-4.832768,-0.057569,1
.045406\C,0,-4.933127,0.99986,-1.112715\C,0,-5.486858,0.09565,-0.18721
\H,0,-5.227119,-0.76856,1.777248\H,0,-5.419145,1.120549,-2.088705\C,0,
-3.273777,2.759519,-1.864496\H,0,-2.403322,3.279166,-1.429152\C,0,-3.0
07677,0.433343,2.735563\C,0,-6.777508,-0.644102,-0.540031\H,0,-6.66175
3,-0.999226,-1.581967\C,0,-3.761402,1.164384,3.867484\H,0,-3.822027,2.
250578,3.684543\H,0,-4.794382,0.779886,3.961037\H,0,-3.252161,1.009994
,4.836863\C,0,-7.977157,0.330447,-0.519255\H,0,-7.811384,1.18772,-1.19
5344\H,0,-8.903918,-0.181964,-0.83701\H,0,-8.137179,0.728496,0.500016\
C,0,-7.063986,-1.869207,0.341518\H,0,-7.298599,-1.576178,1.38148\H,0,-
7.936963,-2.421441,-0.050298\H,0,-6.206056,-2.563067,0.366904\C,0,-2.7
8735,2.048744,-3.14346\H,0,-1.99545,1.320613,-2.902973\H,0,-3.614526,1
.517739,-3.649607\H,0,-2.373838,2.78424,-3.858181\C,0,-4.328912,3.8382
12,-2.184975\H,0,-3.915201,4.589205,-2.882988\H,0,-5.22613,3.398611,-2
.658517\H,0,-4.651896,4.364099,-1.268281\C,0,5.657463,-4.273914,-0.120
181\H,0,5.905676,-4.407796,0.949715\C,0,3.705355,-0.628592,-3.086148\H
,0,3.069521,0.263147,-2.95088\C,0,4.385067,0.179211,1.96528\H,0,3.9483
33,1.14762,1.668081\C,0,4.618019,-5.348931,-0.499383\H,0,4.344002,-5.2
79375,-1.568266\H,0,5.02316,-6.36223,-0.321929\H,0,3.693482,-5.240023,
0.094458\C,0,6.958264,-4.453834,-0.929347\H,0,7.716813,-3.70536,-0.638
293\H,0,7.386646,-5.459387,-0.763033\H,0,6.770703,-4.343125,-2.013344\
C,0,3.455278,-0.432799,3.032859\H,0,3.341773,0.260775,3.886471\H,0,2.4
54289,-0.627922,2.612932\H,0,3.8607,-1.383164,3.425658\C,0,5.786476,0.
475432,2.537658\H,0,6.434547,0.947144,1.777093\H,0,5.715324,1.163426,3
.40019\H,0,6.285545,-0.448575,2.883756\C,0,4.929709,-0.222418,-3.93472
2\H,0,5.592336,-1.091177,-4.107108\H,0,4.610399,0.162757,-4.920841\H,0
,5.527283,0.561941,-3.43878\C,0,2.854756,-1.679631,-3.825247\H,0,2.481
332,-1.258712,-4.777133\H,0,3.439125,-2.584338,-4.074967\H,0,1.984884,

-1.966465,-3.213103\C,0,-2.866788,-1.065159,3.070543\H,0,-2.252765,-1.
193801,3.980628\H,0,-3.846473,-1.539208,3.265339\H,0,-2.373321,-1.6018
01,2.24719\H,0,-1.987271,0.849396,2.676156\C,0,-4.394121,-2.324041,-2.
986389\C,0,-3.072501,-1.897479,-2.728531\H,0,-2.634093,-1.097533,-3.33
3736\C,0,-2.304893,-2.478803,-1.720937\H,0,-1.271177,-2.142405,-1.5911
88\C,0,-2.837648,-3.526686,-0.929372\C,0,-4.15174,-3.977809,-1.20025\H
,0,-4.594004,-4.78209,-0.60497\C,0,-4.915732,-3.374266,-2.203159\H,0,-
5.940741,-3.719286,-2.376736\C,0,-2.042375,-4.16268,0.130858\C,0,-2.31
1137,-5.588349,0.510714\H,0,-1.433386,-6.052906,0.984684\H,0,-2.602451
,-6.16798,-0.378219\H,0,-3.149429,-5.631146,1.230331\N,0,-1.091651,-3.
466703,0.713571\H,0,-0.949884,-2.413026,0.497999\C,0,-0.178668,-3.8934
36,1.730052\C,0,-0.626253,-4.461955,2.93571\H,0,-1.695661,-4.610315,3.
108838\C,0,0.310682,-4.802388,3.921425\H,0,-0.034894,-5.241385,4.86323
8\C,0,1.678544,-4.569771,3.709209\C,0,2.112935,-3.981807,2.509849\H,0,
3.1761,-3.7859,2.342826\C,0,1.18772,-3.629951,1.519087\H,0,1.514046,-3
.161043,0.585996\H,0,2.405947,-4.836384,4.483184\C,0,-5.208387,-1.6695
,-4.07293\H,0,-6.227688,-2.084671,-4.127276\H,0,-5.280418,-0.580559,-3
.89948\H,0,-4.724286,-1.803584,-5.058165\\Version=ES64L-G09RevD.01\Sta
te=1-A\HF=-3216.0905493\RMSD=5.168e-09\Dipole=-2.7069863,-4.2381048,0.
9582992\Quadrupole=0.0261353,18.6984818,-18.7246171,21.4205092,9.55934
68,-10.2331119\PG=C01 [X(C65H72N1O4P1)]\\@

TRIP/1E Switching TS

Conf0

1\1\GINC-WORKER2\SP\RTPSSTPSS\def2SVP\C65H72N1O4P1\JHIOE\26-Mar-2019\0
\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(smd,
solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,0.0347
82,-0.165131,-0.152115\O,0,1.395118,0.615765,0.456654\O,0,-0.826611,1.
19423,-0.662953\O,0,-0.625713,-0.817496,1.040829\O,0,0.317299,-0.97324
3,-1.399012\C,0,1.351228,2.899856,-0.272484\C,0,1.98252,1.65199,-0.235
017\C,0,3.271277,1.411134,-0.807025\C,0,3.900111,2.460424,-1.462631\H,
0,4.897848,2.30996,-1.888631\C,0,3.267375,3.727401,-1.623785\C,0,1.966
006,3.952863,-1.041553\C,0,1.327911,5.207524,-1.281533\H,0,0.323092,5.
377904,-0.884041\C,0,1.95485,6.200821,-2.019577\H,0,1.440723,7.152252,
-2.195457\C,0,3.253765,5.991777,-2.555978\H,0,3.741232,6.786757,-3.130
902\C,0,3.891614,4.776185,-2.364417\H,0,4.884909,4.594878,-2.791038\C,
0,0.077948,3.091445,0.478858\C,0,-0.988481,2.214664,0.25447\C,0,-2.264
24,2.35618,0.888059\C,0,-2.43437,3.41356,1.771162\H,0,-3.410905,3.5740
55,2.239146\C,0,-1.364094,4.29248,2.107361\C,0,-0.078521,4.122575,1.47
5144\C,0,0.995639,4.964708,1.895611\H,0,1.988817,4.819931,1.461124\C,0
,0.801391,5.949359,2.853338\H,0,1.643463,6.578019,3.163334\C,0,-0.4771
45,6.14448,3.441148\H,0,-0.618867,6.930265,4.191178\C,0,-1.535202,5.32
691,3.076404\H,0,-2.520897,5.451176,3.539352\C,0,-3.380599,1.409513,0.
556978\C,0,-3.766417,0.39074,1.473954\C,0,-4.060068,1.541095,-0.681035
\C,0,-4.831272,-0.456868,1.126023\C,0,-5.116217,0.657797,-0.986085\C,0
,-5.522174,-0.349607,-0.096511\H,0,-5.140171,-1.234339,1.834327\H,0,-5
.62806,0.773603,-1.946566\C,0,3.899003,0.058863,-0.662256\C,0,4.021328
,-0.801348,-1.788542\C,0,4.356021,-0.370854,0.612701\C,0,4.60803,-2.06
8321,-1.614431\C,0,4.942555,-1.644713,0.731872\C,0,5.075215,-2.512328,
-0.364831\H,0,4.701351,-2.729243,-2.484023\H,0,5.307356,-1.974821,1.71
234\C,0,4.252301,0.517971,1.85379\H,0,3.74548,1.452205,1.559324\C,0,3.
544717,-0.389383,-3.183504\C,0,5.702382,-3.89393,-0.198682\H,0,5.97310
2,-4.000099,0.869016\C,0,4.745837,-0.116287,-4.112977\H,0,5.415963,0.6
54386,-3.691807\H,0,5.343173,-1.034112,-4.267986\H,0,4.40043,0.234442,
-5.103072\C,0,6.996515,-4.031905,-1.026487\H,0,7.724794,-3.243881,-0.7
63606\H,0,7.472893,-5.013473,-0.847739\H,0,6.786657,-3.952557,-2.10918
6\C,0,4.70201,-5.016596,-0.543161\H,0,4.404266,-4.972532,-1.607003\H,0
,5.151955,-6.009949,-0.361031\H,0,3.785583,-4.937176,0.067758\C,0,3.39
9063,-0.136749,2.959014\H,0,2.398116,-0.396808,2.577222\H,0,3.877927,-
1.054359,3.34563\H,0,3.274246,0.558682,3.809561\C,0,5.649321,0.909516,
2.378967\H,0,5.560817,1.601657,3.236598\H,0,6.215387,0.022441,2.718622
\H,0,6.243485,1.41232,1.594725\C,0,-6.657383,-1.332812,-0.396569\H,0,-
7.316098,-1.327375,0.494822\C,0,-3.074852,0.218841,2.828633\H,0,-2.080
942,0.689451,2.742991\C,0,-3.68988,2.637435,-1.682661\H,0,-2.858451,3.
218999,-1.249717\C,0,-7.51647,-0.947716,-1.610518\H,0,-6.935192,-0.992
848,-2.549846\H,0,-8.364331,-1.648107,-1.713818\H,0,-7.929611,0.072226
,-1.513456\C,0,-6.119704,-2.774612,-0.547685\H,0,-5.534566,-3.081992,0
.336493\H,0,-6.955354,-3.488622,-0.666636\H,0,-5.467257,-2.859491,-1.4
34175\C,0,-3.189011,2.056534,-3.019389\H,0,-2.843159,2.868476,-3.68534
1\H,0,-2.34572,1.36506,-2.854252\H,0,-3.994048,1.51418,-3.548327\C,0,-
4.86001,3.618404,-1.900332\H,0,-5.186075,4.06813,-0.945194\H,0,-4.5578
04,4.437516,-2.578665\H,0,-5.73219,3.111763,-2.353347\C,0,-3.863027,0.
936457,3.946023\H,0,-4.8677,0.488842,4.064869\H,0,-3.334414,0.847131,4
.91321\H,0,-3.997567,2.00997,3.730229\C,0,-2.842238,-1.257976,3.201445
\H,0,-2.220855,-1.323161,4.113605\H,0,-3.789612,-1.787703,3.413655\H,0

,-2.307888,-1.777944,2.39209\C,0,2.580322,-1.420625,-3.802364\H,0,2.22
5823,-1.06323,-4.787197\H,0,3.071073,-2.398414,-3.963239\H,0,1.705131,
-1.560087,-3.146214\H,0,2.981548,0.553464,-3.079022\C,0,1.695809,-3.94
1035,3.341706\C,0,0.443036,-4.459186,3.7391\H,0,0.310871,-4.824163,4.7
63591\C,0,-0.632039,-4.511891,2.850791\H,0,-1.59072,-4.906073,3.198842
\C,0,-0.496914,-4.023504,1.527638\C,0,0.761401,-3.505219,1.125875\H,0,
0.914965,-3.148088,0.1024\C,0,1.83326,-3.476085,2.015819\H,0,2.794403,
-3.078829,1.676271\C,0,-1.61377,-4.059379,0.582176\C,0,-2.721921,-5.05
2504,0.728196\H,0,-3.023038,-5.101359,1.787457\H,0,-2.373688,-6.062608
,0.446811\H,0,-3.59717,-4.787234,0.118716\N,0,-1.604478,-3.176801,-0.4
02341\H,0,-0.943675,-2.378492,-0.295389\C,0,-2.405532,-3.118456,-1.578
136\C,0,-2.714378,-4.282657,-2.308361\H,0,-2.345675,-5.25665,-1.976569
\C,0,-3.462007,-4.1758,-3.487633\H,0,-3.698474,-5.080465,-4.057323\C,0
,-3.885232,-2.918264,-3.946674\C,0,-3.556632,-1.762349,-3.22084\H,0,-3
.886226,-0.780616,-3.570546\C,0,-2.818399,-1.852728,-2.035451\H,0,-2.5
84749,-0.954714,-1.458357\H,0,-4.464254,-2.838021,-4.872534\C,0,2.8455
43,-3.856436,4.31255\H,0,2.80809,-4.668387,5.058555\H,0,3.816575,-3.89
1144,3.791147\H,0,2.800106,-2.898729,4.866083\\Version=ES64L-G09RevD.0
1\State=1-A\HF=-3216.0860407\RMSD=4.893e-09\Dipole=-1.7733435,-4.49895
5,0.994833\Quadrupole=-9.1398178,22.5881989,-13.4483811,16.5807397,9.9
252408,-8.5907668\PG=C01 [X(C65H72N1O4P1)]\\@

Conf1

1\1\GINC-WORKER1\SP\RTPSSTPSS\def2SVP\C65H72N1O4P1\JHIOE\29-Mar-2019\0
\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(smd,
solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,0.0317
69,-0.176859,-0.219803\O,0,1.418689,0.536058,0.414616\O,0,-0.77859,1.2
27426,-0.690323\O,0,-0.657435,-0.838211,0.951711\O,0,0.289369,-0.95859
9,-1.488712\C,0,1.427718,2.8595,-0.184595\C,0,2.027652,1.595618,-0.220
777\C,0,3.305467,1.355583,-0.817287\C,0,3.958949,2.425167,-1.413022\H,
0,4.949277,2.273806,-1.855198\C,0,3.36249,3.716958,-1.490768\C,0,2.069
433,3.941388,-0.890402\C,0,1.466791,5.226079,-1.051805\H,0,0.467383,5.
400853,-0.643326\C,0,2.120949,6.245672,-1.727772\H,0,1.633384,7.220135
,-1.842413\C,0,3.412696,6.034509,-2.280165\H,0,3.921687,6.849789,-2.80
5861\C,0,4.01511,4.791424,-2.167589\H,0,5.001546,4.607846,-2.608852\C,
0,0.151002,3.039016,0.564578\C,0,-0.933646,2.20553,0.273144\C,0,-2.219
242,2.350659,0.885529\C,0,-2.382197,3.368657,1.81478\H,0,-3.36535,3.53
3898,2.267031\C,0,-1.297018,4.201135,2.215762\C,0,-0.001497,4.024943,1
.606142\C,0,1.083054,4.819839,2.08732\H,0,2.082047,4.667534,1.668912\C
,0,0.890747,5.767804,3.081726\H,0,1.740392,6.361331,3.437034\C,0,-0.39
6159,5.970708,3.648342\H,0,-0.53602,6.727629,4.42783\C,0,-1.464912,5.1
95814,3.226108\H,0,-2.457912,5.325233,3.671714\C,0,-3.352219,1.453263,
0.482006\C,0,-3.792002,0.405462,1.339442\C,0,-3.9883,1.660205,-0.77054
8\C,0,-4.860597,-0.406805,0.918768\C,0,-5.058308,0.823355,-1.140625\C,
0,-5.507103,-0.22057,-0.316219\H,0,-5.197592,-1.214768,1.577085\H,0,-5
.551423,0.983291,-2.107331\C,0,3.903399,-0.017518,-0.766061\C,0,3.9709
47,-0.812691,-1.941039\C,0,4.40067,-0.524261,0.466075\C,0,4.560196,-2.
089954,-1.861773\C,0,4.975281,-1.807303,0.493793\C,0,5.070629,-2.60722
1,-0.660003\H,0,4.623361,-2.705063,-2.767682\H,0,5.365395,-2.190344,1.
444285\C,0,4.357283,0.301453,1.753497\H,0,3.848425,1.253785,1.528653\C
,0,3.440335,-0.312001,-3.286507\C,0,5.712154,-3.991781,-0.614583\H,0,5
.680149,-4.396117,-1.64385\C,0,4.603326,0.083266,-4.220875\H,0,5.25587
3,0.843292,-3.755822\H,0,5.229848,-0.795026,-4.464616\H,0,4.216434,0.4
98584,-5.169825\C,0,4.922722,-4.959261,0.290654\H,0,3.869614,-5.038007
,-0.031395\H,0,5.367368,-5.97097,0.260701\H,0,4.932929,-4.619604,1.342
57\C,0,7.192418,-3.916265,-0.187495\H,0,7.291203,-3.537955,0.846804\H,
0,7.661464,-4.916648,-0.225796\H,0,7.765636,-3.243685,-0.850572\C,0,3.
544401,-0.400309,2.859068\H,0,2.519853,-0.616916,2.514056\H,0,4.019624
,-1.349191,3.165135\H,0,3.477686,0.243446,3.755562\C,0,5.780356,0.6526
68,2.235756\H,0,5.738351,1.300315,3.130904\H,0,6.350539,-0.256314,2.50
3376\H,0,6.344955,1.188862,1.45175\C,0,-6.670022,-1.112285,-0.74439\H,
0,-6.890206,-0.869458,-1.801149\C,0,-3.152729,0.159865,2.708082\H,0,-2
.149681,0.618015,2.682671\C,0,-3.548256,2.776538,-1.719625\H,0,-2.7021
25,3.303745,-1.247493\C,0,-6.318569,-2.612033,-0.673633\H,0,-6.129279,
-2.933688,0.366825\H,0,-7.152928,-3.222678,-1.064329\H,0,-5.418552,-2.
838767,-1.270658\C,0,-7.935839,-0.801937,0.081586\H,0,-8.219776,0.2618
83,-0.007334\H,0,-8.789167,-1.41559,-0.261722\H,0,-7.77002,-1.020259,1
.15294\C,0,-3.043701,2.219374,-3.0655\H,0,-2.652124,3.037291,-3.698015
\H,0,-2.231928,1.48962,-2.906314\H,0,-3.857571,1.72504,-3.627002\C,0,-
4.668983,3.815858,-1.923816\H,0,-4.995392,4.243633,-0.95876\H,0,-4.315
855,4.645185,-2.564017\H,0,-5.552674,3.365957,-2.413032\C,0,-3.974209,
0.837952,3.826372\H,0,-4.988564,0.400581,3.885857\H,0,-3.484975,0.6975
31,4.808128\H,0,-4.086523,1.921968,3.654658\C,0,-2.954855,-1.335526,3.
021406\H,0,-2.374806,-1.450346,3.955533\H,0,-3.916381,-1.862265,3.1665
36\H,0,-2.390611,-1.823382,2.212641\C,0,2.49795,-1.32398,-3.967179\H,0
,2.096281,-0.893698,-4.903479\H,0,3.020903,-2.260833,-4.234265\H,0,1.6
50249,-1.558023,-3.302213\H,0,2.845796,0.596007,-3.087808\C,0,1.603097

,-4.024179,3.193087\C,0,0.342626,-4.525481,3.587529\H,0,0.207476,-4.90
1958,4.607467\C,0,-0.736852,-4.544562,2.703305\H,0,-1.701875,-4.922286
,3.051638\C,0,-0.59754,-4.041606,1.386019\C,0,0.669637,-3.543003,0.986
744\H,0,0.826488,-3.175166,-0.032372\C,0,1.744486,-3.543804,1.873064\H
,0,2.711314,-3.160924,1.534453\C,0,-1.721413,-4.034314,0.448466\C,0,-2
.860233,-4.9931,0.591063\H,0,-3.139041,-5.068198,1.654539\H,0,-2.55443
3,-6.004348,0.267203\H,0,-3.739239,-4.676209,0.011601\N,0,-1.692569,-3
.14139,-0.526797\H,0,-1.008789,-2.363599,-0.414938\C,0,-2.505693,-3.04
1688,-1.691237\C,0,-2.863484,-4.184849,-2.43272\H,0,-2.521768,-5.17525
7,-2.121227\C,0,-3.62703,-4.036466,-3.597119\H,0,-3.902376,-4.924547,-
4.175401\C,0,-4.01705,-2.759369,-4.03129\C,0,-3.63766,-1.62511,-3.2964
49\H,0,-3.937307,-0.627243,-3.62775\C,0,-2.882816,-1.756737,-2.125471\
H,0,-2.609138,-0.874688,-1.541526\H,0,-4.60845,-2.647448,-4.946003\C,0
,2.756291,-3.972974,4.161942\H,0,2.70557,-4.793067,4.898135\H,0,3.7251
82,-4.018971,3.637602\H,0,2.7306,-3.021276,4.726917\\Version=ES64L-G09
RevD.01\State=1-A\HF=-3216.0871784\RMSD=4.771e-09\Dipole=-1.8566272,-4
.4193497,0.9127594\Quadrupole=-7.758896,21.7723652,-14.0134691,16.7206
18,11.2113056,-7.0648878\PG=C01 [X(C65H72N1O4P1)]\\@

Conf2

1\1\GINC-WORKER2\SP\RTPSSTPSS\def2SVP\C65H72N1O4P1\JHIOE\01-Apr-2019\0
\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(smd,
solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,0.0593
84,-0.178424,-0.168572\O,0,1.407615,0.596532,0.472944\O,0,-0.788341,1.
18385,-0.696524\O,0,-0.629622,-0.83046,1.008195\O,0,0.367884,-0.985082
,-1.410367\C,0,1.36528,2.895659,-0.207176\C,0,2.002058,1.650386,-0.184
761\C,0,3.303145,1.428222,-0.735448\C,0,3.942329,2.495551,-1.350364\H,
0,4.949772,2.35926,-1.757751\C,0,3.309841,3.765133,-1.490316\C,0,1.994
381,3.971138,-0.933112\C,0,1.358419,5.230356,-1.154738\H,0,0.343398,5.
387445,-0.778416\C,0,2.000355,6.245544,-1.848863\H,0,1.487611,7.20018,
-2.010856\C,0,3.312937,6.05511,-2.358089\H,0,3.812246,6.867269,-2.8977
22\C,0,3.949151,4.835888,-2.185412\H,0,4.953183,4.668718,-2.592179\C,0
,0.069431,3.062647,0.51113\C,0,-0.987229,2.19082,0.22866\C,0,-2.288147
,2.325085,0.810449\C,0,-2.491111,3.361772,1.710771\H,0,-3.486355,3.516
134,2.139844\C,0,-1.432644,4.228362,2.110727\C,0,-0.124308,4.071169,1.
523827\C,0,0.933326,4.903132,2.002336\H,0,1.94193,4.766814,1.601867\C,
0,0.703664,5.865847,2.974435\H,0,1.533477,6.486941,3.329554\C,0,-0.595
851,6.048306,3.518809\H,0,-0.765219,6.816877,4.280884\C,0,-1.639482,5.
239594,3.097112\H,0,-2.641877,5.353921,3.525452\C,0,-3.396826,1.399765
,0.40194\C,0,-3.829426,0.353548,1.264598\C,0,-4.019825,1.581873,-0.861
244\C,0,-4.876005,-0.483974,0.838089\C,0,-5.06844,0.720453,-1.236725\C
,0,-5.508951,-0.323054,-0.407355\H,0,-5.206752,-1.291104,1.500541\H,0,
-5.551177,0.860569,-2.21171\C,0,3.934199,0.075608,-0.609036\C,0,4.0667
37,-0.765296,-1.748403\C,0,4.385708,-0.371796,0.66125\C,0,4.661358,-2.
030851,-1.592076\C,0,4.980983,-1.643248,0.762932\C,0,5.12595,-2.491444
,-0.347255\H,0,4.76414,-2.677203,-2.471466\H,0,5.342316,-1.987001,1.74
0004\C,0,4.261952,0.493988,1.916572\H,0,3.748037,1.428137,1.634172\C,0
,3.596695,-0.327772,-3.137765\C,0,5.761417,-3.871489,-0.200166\H,0,6.0
33239,-3.990468,0.865893\C,0,4.802876,0.005496,-4.040745\H,0,5.444785,
0.781757,-3.587479\H,0,5.427714,-0.890785,-4.212417\H,0,4.462042,0.375
007,-5.025603\C,0,7.05599,-3.991815,-1.0301\H,0,7.780342,-3.203439,-0.
75757\H,0,7.537602,-4.973059,-0.863957\H,0,6.845478,-3.899986,-2.11168
4\C,0,4.767129,-4.995059,-0.559432\H,0,4.468007,-4.937623,-1.622268\H,
0,5.223055,-5.988251,-0.391784\H,0,3.850796,-4.929814,0.053311\C,0,3.4
044,-0.189392,3.000841\H,0,2.409283,-0.451294,2.604905\H,0,3.887831,-1
.110053,3.374104\H,0,3.265343,0.488442,3.863327\C,0,5.649569,0.890067,
2.462295\H,0,5.545615,1.561626,3.33439\H,0,6.223325,0.002293,2.786925\
H,0,6.243891,1.41705,1.694209\C,0,-6.65117,-1.239166,-0.840045\H,0,-6.
861622,-1.012791,-1.902414\C,0,-3.206157,0.137465,2.645603\H,0,-2.2080
25,0.606583,2.626411\C,0,-3.585304,2.693697,-1.818403\H,0,-2.768753,3.
254276,-1.332685\C,0,-6.278446,-2.732477,-0.745946\H,0,-6.092528,-3.03
7084,0.30025\H,0,-7.101377,-3.360074,-1.134111\H,0,-5.371325,-2.955001
,-1.333782\C,0,-7.932266,-0.937792,-0.034201\H,0,-8.229677,0.120913,-0
.138796\H,0,-8.772387,-1.56716,-0.381588\H,0,-7.777501,-1.141939,1.041
602\C,0,-3.023956,2.124517,-3.136717\H,0,-2.634621,2.940279,-3.773441\
H,0,-2.198417,1.420538,-2.937567\H,0,-3.806419,1.597134,-3.712728\C,0,
-4.72824,3.695899,-2.07815\H,0,-5.094933,4.135389,-1.133053\H,0,-4.379
212,4.52055,-2.726533\H,0,-5.584175,3.211168,-2.582987\C,0,-4.050993,0
.823358,3.741402\H,0,-5.06143,0.376043,3.792683\H,0,-3.57482,0.702645,
4.732156\H,0,-4.171827,1.903442,3.551841\C,0,-2.995601,-1.350342,2.985
141\H,0,-2.422582,-1.444632,3.925803\H,0,-3.953027,-1.884568,3.12973\H
,0,-2.419133,-1.845171,2.18948\C,0,2.669707,-1.364942,-3.801894\H,0,2.
316598,-0.985053,-4.778719\H,0,3.189399,-2.322775,-3.989439\H,0,1.7909
1,-1.549867,-3.162014\H,0,3.006888,0.596385,-3.013297\C,0,1.714114,-3.
994284,3.29239\C,0,0.459589,-4.508249,3.689444\H,0,0.329566,-4.883895,
4.710342\C,0,-0.619923,-4.543322,2.805653\H,0,-1.579695,-4.933607,3.15
477\C,0,-0.487006,-4.043876,1.486402\C,0,0.773095,-3.528768,1.085396\H

,0,0.925784,-3.161369,0.065405\C,0,1.848407,-3.514136,1.971468\H,0,2.8
10279,-3.118317,1.632115\C,0,-1.608116,-4.063051,0.545368\C,0,-2.73470
5,-5.034879,0.695665\H,0,-3.018199,-5.09724,1.758772\H,0,-2.414735,-6.
046964,0.38865\H,0,-3.614794,-4.738029,0.107184\N,0,-1.588418,-3.18096
7,-0.439579\H,0,-0.916432,-2.392153,-0.334638\C,0,-2.39385,-3.108225,-
1.611039\C,0,-2.725231,-4.266461,-2.341309\H,0,-2.373131,-5.247102,-2.
011142\C,0,-3.473659,-4.145245,-3.518506\H,0,-3.727896,-5.045003,-4.08
8321\C,0,-3.874539,-2.879726,-3.976092\C,0,-3.523811,-1.730454,-3.2504
31\H,0,-3.833818,-0.741908,-3.599123\C,0,-2.785743,-1.834918,-2.066036
\H,0,-2.534929,-0.941253,-1.48914\H,0,-4.452985,-2.788534,-4.901331\C,
0,2.868934,-3.931179,4.258693\H,0,2.834331,-4.758753,4.987529\H,0,3.83
7119,-3.955825,3.731606\H,0,2.827342,-2.985866,4.833379\\Version=ES64L
-G09RevD.01\State=1-A\HF=-3216.0870195\RMSD=4.730e-09\Dipole=-1.791023
9,-4.4433182,0.9519908\Quadrupole=-9.1511528,22.5402497,-13.3890968,16
.0129477,11.0477293,-8.3206864\PG=C01 [X(C65H72N1O4P1)]\\@

Conf3

1\1\GINC-WORKER0\SP\RTPSSTPSS\def2SVP\C65H72N1O4P1\JHIOE\29-Apr-2019\0
\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(smd,
solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,0.0226
98,-0.175332,-0.184181\O,0,1.414735,0.560129,0.410699\O,0,-0.820413,1.
21519,-0.638\O,0,-0.624708,-0.844138,1.006991\O,0,0.257783,-0.957818,-
1.456772\C,0,1.385562,2.87523,-0.217747\C,0,1.997437,1.617185,-0.25297
1\C,0,3.262497,1.382103,-0.878053\C,0,3.89088,2.451192,-1.501437\H,0,4
.871139,2.303636,-1.966944\C,0,3.279304,3.735881,-1.580342\C,0,1.99811
9,3.954072,-0.952957\C,0,1.376641,5.229402,-1.116833\H,0,0.384747,5.39
7377,-0.687431\C,0,2.003477,6.247501,-1.820311\H,0,1.502302,7.214859,-
1.936564\C,0,3.284929,6.043727,-2.398994\H,0,3.772701,6.857941,-2.9460
39\C,0,3.904195,4.809053,-2.284793\H,0,4.882379,4.631171,-2.746342\C,0
,0.128831,3.052571,0.564631\C,0,-0.954966,2.203243,0.318247\C,0,-2.222
348,2.34322,0.968568\C,0,-2.368385,3.37376,1.886933\H,0,-3.338664,3.53
4755,2.367619\C,0,-1.280478,4.222456,2.243708\C,0,-0.002078,4.050364,1
.597916\C,0,1.089007,4.860439,2.037437\H,0,2.076709,4.711781,1.591893\
C,0,0.917359,5.818902,3.025522\H,0,1.771796,6.423787,3.348685\C,0,-0.3
54205,6.017998,3.627006\H,0,-0.478075,6.783429,4.400862\C,0,-1.428008,
5.22922,3.245268\H,0,-2.408593,5.355821,3.71831\C,0,-3.356291,1.423962
,0.621108\C,0,-3.755861,0.392987,1.518323\C,0,-4.041019,1.595248,-0.60
902\C,0,-4.840773,-0.424593,1.160731\C,0,-5.118109,0.741475,-0.92445\C
,0,-5.538746,-0.276251,-0.053492\H,0,-5.160246,-1.210433,1.855016\H,0,
-5.634674,0.889132,-1.878035\C,0,3.872257,0.014357,-0.830574\C,0,3.935
891,-0.780865,-2.005957\C,0,4.384181,-0.488826,0.397494\C,0,4.534807,-
2.053939,-1.931494\C,0,4.966817,-1.768214,0.420356\C,0,5.057545,-2.568
05,-0.733937\H,0,4.593146,-2.669014,-2.837826\H,0,5.367708,-2.148658,1
.367376\C,0,4.352481,0.337978,1.684681\H,0,3.832692,1.28589,1.466463\C
,0,3.384076,-0.29134,-3.347017\C,0,5.70709,-3.948943,-0.693092\H,0,5.6
6489,-4.355884,-1.720958\C,0,4.529489,0.073515,-4.314423\H,0,5.203247,
0.83126,-3.876298\H,0,5.138233,-0.816412,-4.560869\H,0,4.125415,0.4805
31,-5.259799\C,0,4.933916,-4.917921,0.224457\H,0,3.876801,-5.001589,-0
.083009\H,0,5.382339,-5.92782,0.19062\H,0,4.957248,-4.575659,1.275309\
C,0,7.191931,-3.864508,-0.283685\H,0,7.30056,-3.482589,0.748302\H,0,7.
665738,-4.862549,-0.324549\H,0,7.753943,-3.190911,-0.955254\C,0,3.5625
51,-0.367966,2.804204\H,0,2.534858,-0.593714,2.475306\H,0,4.050325,-1.
311918,3.106326\H,0,3.504125,0.277931,3.699732\C,0,5.780053,0.701139,2
.144904\H,0,5.746437,1.349391,3.039993\H,0,6.361233,-0.203123,2.404771
\H,0,6.329013,1.240735,1.352188\C,0,-6.696879,-1.228492,-0.365683\H,0,
-7.352776,-1.222909,0.527859\C,0,-3.057877,0.176328,2.863261\H,0,-2.06
2315,0.645083,2.787547\C,0,-3.655881,2.706413,-1.5881\H,0,-2.800953,3.
252256,-1.154513\C,0,-7.550414,-0.804829,-1.570514\H,0,-6.972458,-0.84
8136,-2.51199\H,0,-8.414159,-1.484254,-1.682112\H,0,-7.9404,0.222417,-
1.456354\C,0,-6.19186,-2.679196,-0.542439\H,0,-5.612367,-3.01459,0.335
216\H,0,-7.043364,-3.372161,-0.672438\H,0,-5.542803,-2.76324,-1.431493
\C,0,-3.195523,2.148366,-2.948748\H,0,-2.839631,2.968267,-3.599457\H,0
,-2.368508,1.43032,-2.817944\H,0,-4.024321,1.642149,-3.476789\C,0,-4.8
01259,3.725296,-1.757083\H,0,-5.097567,4.156079,-0.783674\H,0,-4.48831
3,4.5549,-2.417575\H,0,-5.695347,3.255764,-2.2075\C,0,-3.837346,0.8629
86,4.005886\H,0,-4.842902,0.41549,4.117454\H,0,-3.303744,0.743866,4.96
7104\H,0,-3.969523,1.942804,3.821961\C,0,-2.828442,-1.312272,3.187805\
H,0,-2.212493,-1.407995,4.100999\H,0,-3.776936,-1.849073,3.375785\H,0,
-2.288774,-1.803359,2.364115\C,0,2.412359,-1.302051,-3.987536\H,0,1.99
6332,-0.884627,-4.923432\H,0,2.916327,-2.251664,-4.246167\H,0,1.576813
,-1.511465,-3.299229\H,0,2.806208,0.627495,-3.150008\C,0,1.657311,-4.0
19332,3.230933\C,0,0.403281,-4.52914,3.634918\H,0,0.278225,-4.906442,4
.655821\C,0,-0.682356,-4.556741,2.758265\H,0,-1.641896,-4.942817,3.112
657\C,0,-0.556275,-4.051905,1.440468\C,0,0.704088,-3.543906,1.031763\H
,0,0.850396,-3.17452,0.01168\C,0,1.78564,-3.538669,1.909756\H,0,2.7476
45,-3.150587,1.563762\C,0,-1.68594,-4.055099,0.509686\C,0,-2.809261,-5
.031415,0.654472\H,0,-3.098234,-5.092764,1.716474\H,0,-2.481938,-6.042

454,0.352023\H,0,-3.687362,-4.740816,0.060796\N,0,-1.674842,-3.156892,
-0.460701\H,0,-0.99934,-2.371548,-0.349809\C,0,-2.491374,-3.064009,-1.
623627\C,0,-2.829072,-4.208652,-2.371927\H,0,-2.472392,-5.195044,-2.06
4227\C,0,-3.590175,-4.066364,-3.538836\H,0,-3.84923,-4.955711,-4.12266
2\C,0,-3.997922,-2.793293,-3.968148\C,0,-3.64055,-1.65731,-3.224696\H,
0,-3.957469,-0.66345,-3.551094\C,0,-2.888572,-1.783083,-2.051299\H,0,-
2.632593,-0.900527,-1.460074\H,0,-4.587432,-2.685425,-4.884529\C,0,2.8
18392,-3.959398,4.189892\H,0,2.769065,-4.767088,4.939662\H,0,3.782777,
-4.020001,3.658454\H,0,2.80362,-2.998071,4.738813\\Version=ES64L-G09Re
vD.01\State=1-A\HF=-3216.0861985\RMSD=4.937e-09\Dipole=-1.8123446,-4.4
787249,0.9611602\Quadrupole=-7.8820823,22.2282103,-14.3461281,16.69278
15,10.0588739,-7.6403088\PG=C01 [X(C65H72N1O4P1)]\\@

TRIP/2E Type I

Conf0
1\1\GINC-WORKER0\SP\RTPSSTPSS\def2SVP\C65H69F3N1O4P1\JHIOE\07-May-2019
\0\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(sm
d,solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,0.19
0648,-0.599056,-1.387063\O,0,-1.128743,0.348037,-1.786618\O,0,0.968308
,0.458384,-0.312399\O,0,0.959487,-0.804237,-2.658069\O,0,-0.219947,-1.
741798,-0.460601\C,0,-1.235505,2.217502,-0.291974\C,0,-1.819331,1.0688
67,-0.834822\C,0,-3.151846,0.646063,-0.528005\C,0,-3.877778,1.401982,0
.38302\H,0,-4.907586,1.115694,0.621441\C,0,-3.308486,2.526644,1.046955
\C,0,-1.959628,2.931552,0.732511\C,0,-1.382377,3.995808,1.489673\H,0,-
0.345155,4.285256,1.298847\C,0,-2.108892,4.651208,2.473021\H,0,-1.6386
51,5.456918,3.047496\C,0,-3.4525,4.281289,2.747339\H,0,-4.015859,4.808
435,3.524856\C,0,-4.035446,3.236125,2.049659\H,0,-5.058803,2.917101,2.
275834\C,0,0.115085,2.657764,-0.746825\C,0,1.191735,1.766732,-0.692677
\C,0,2.546155,2.162107,-0.922713\C,0,2.783625,3.473773,-1.308423\H,0,3
.812509,3.811606,-1.469607\C,0,1.718568,4.399649,-1.507265\C,0,0.36162
3,3.993339,-1.233828\C,0,-0.686074,4.930548,-1.484625\H,0,-1.723903,4.
626345,-1.320906\C,0,-0.408344,6.208754,-1.946547\H,0,-1.2308,6.906701
,-2.138303\C,0,0.931772,6.618026,-2.180498\H,0,1.138282,7.632498,-2.53
8703\C,0,1.971389,5.725923,-1.970578\H,0,3.008575,6.0221,-2.165085\C,0
,-1.840767,-0.32622,4.222974\C,0,-1.411562,-1.484586,4.888998\H,0,-1.9
03548,-1.804252,5.811275\C,0,-0.349623,-2.230366,4.366465\H,0,-0.02470
7,-3.135077,4.887599\C,0,0.264,-1.842085,3.154865\C,0,-0.168735,-0.665
363,2.502005\H,0,0.321572,-0.321303,1.588773\C,0,-1.211234,0.090163,3.
037115\H,0,-1.535486,1.00229,2.529181\C,0,1.361662,-2.659383,2.593705\
C,0,2.321206,-3.336595,3.522438\H,0,3.295159,-3.50816,3.038505\H,0,1.9
16938,-4.316567,3.836945\H,0,2.454501,-2.72451,4.427382\N,0,1.469968,-
2.736667,1.289386\H,0,0.742524,-2.238373,0.65165\C,0,2.427017,-3.47187
7,0.520809\C,0,3.003219,-2.823454,-0.587703\H,0,2.779532,-1.773753,-0.
794647\C,0,3.890291,-3.529497,-1.408809\H,0,4.34505,-3.019928,-2.26317
\C,0,4.199673,-4.870454,-1.132929\C,0,3.612944,-5.512044,-0.030378\H,0
,3.838747,-6.562245,0.181649\C,0,2.718924,-4.820902,0.79776\H,0,2.2266
87,-5.333471,1.628055\C,0,3.659037,1.189295,-0.670731\C,0,4.352209,0.5
83344,-1.749856\C,0,4.012893,0.877035,0.673051\C,0,5.405428,-0.307483,
-1.461655\C,0,5.063731,-0.025715,0.906091\C,0,5.773365,-0.632236,-0.14
6852\H,0,5.947451,-0.779771,-2.289265\H,0,5.338491,-0.264013,1.938324\
C,0,-3.729094,-0.562236,-1.200017\C,0,-4.029362,-1.729752,-0.446566\C,
0,-3.981801,-0.540356,-2.601831\C,0,-4.585964,-2.841793,-1.109176\C,0,
-4.534579,-1.677918,-3.213602\C,0,-4.845256,-2.841957,-2.487905\H,0,-4
.817012,-3.744788,-0.530598\H,0,-4.733014,-1.652777,-4.291564\H,0,4.89
4103,-5.417168,-1.779403\C,0,-2.996181,0.489098,4.74941\C,0,-3.7145,0.
697306,-3.462025\H,0,-3.25376,1.467185,-2.821047\C,0,-3.749299,-1.8373
85,1.05382\C,0,-5.438411,-4.068184,-3.17656\H,0,-5.586646,-4.838385,-2
.396343\C,0,-5.058437,-1.92374,1.864656\H,0,-4.844969,-1.978576,2.9470
28\H,0,-5.69833,-1.040966,1.688183\H,0,-5.638966,-2.82354,1.588486\C,0
,-4.470569,-4.64781,-4.228872\H,0,-4.288688,-3.924682,-5.045211\H,0,-3
.49452,-4.900695,-3.777744\H,0,-4.888957,-5.566424,-4.68001\C,0,-6.815
776,-3.761287,-3.799602\H,0,-7.253645,-4.673354,-4.245347\H,0,-7.52154
2,-3.377969,-3.040877\H,0,-6.733175,-3.00231,-4.599533\C,0,-2.725395,0
.402374,-4.608182\H,0,-3.14347,-0.327662,-5.325828\H,0,-2.501505,1.328
896,-5.168535\H,0,-1.776451,0.001859,-4.214463\C,0,-5.03397,1.291492,-
3.998987\H,0,-4.837824,2.218726,-4.568504\H,0,-5.548725,0.583509,-4.67
4495\H,0,-5.726085,1.537107,-3.173236\C,0,6.919963,-1.603488,0.122168\
H,0,7.123984,-2.130401,-0.829283\C,0,3.987681,0.885684,-3.204212\H,0,2
.990965,1.359376,-3.196844\C,0,3.299496,1.549604,1.849073\H,0,2.255573
,1.733762,1.540852\C,0,8.201439,-0.8381,0.516324\H,0,9.045477,-1.53594
2,0.668679\H,0,8.490434,-0.114725,-0.26684\H,0,8.049393,-0.276974,1.45
7175\C,0,6.565618,-2.669149,1.177847\H,0,6.425515,-2.220902,2.17847\H,
0,5.638119,-3.204747,0.909755\H,0,7.379221,-3.412605,1.259663\C,0,3.24
6036,0.681159,3.117744\H,0,2.876225,-0.333317,2.893408\H,0,4.237567,0.
583409,3.596178\H,0,2.565893,1.135842,3.859646\C,0,3.935759,2.923263,2

.155403\H,0,3.917824,3.580376,1.268542\H,0,3.389145,3.433154,2.970107\
H,0,4.988897,2.803109,2.470059\C,0,4.989169,1.886242,-3.819271\H,0,5.0
32813,2.82437,-3.238802\H,0,6.008305,1.456959,-3.843238\H,0,4.701643,2
.138688,-4.856671\C,0,3.873197,-0.383639,-4.070038\H,0,3.531704,-0.112
802,-5.086175\H,0,4.843729,-0.901641,-4.178079\H,0,3.133442,-1.076725,
-3.638535\C,0,-2.81164,-3.018736,1.377231\H,0,-3.286722,-3.991075,1.15
0501\H,0,-1.879085,-2.937932,0.79484\H,0,-2.554352,-3.015583,2.452041\
H,0,-3.226223,-0.91917,1.365743\F,0,-2.647595,1.786384,4.953087\F,0,-4
.035356,0.505682,3.866125\F,0,-3.484097,0.017696,5.92033\\Version=ES64
L-G09RevD.01\State=1-A\HF=-3513.6183668\RMSD=2.003e-09\Dipole=2.580562
6,-2.8086783,4.6444803\Quadrupole=-7.9075191,17.3759406,-9.4684214,-16
.2257663,8.8167536,-23.2629552\PG=C01 [X(C65H69F3N1O4P1)]\\@

Conf1

1\1\GINC-WORKER1\SP\RTPSSTPSS\def2SVP\C65H69F3N1O4P1\JHIOE\07-May-2019
\0\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(sm
d,solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,0.20
0875,-0.478127,-1.498589\O,0,-1.097342,0.512456,-1.861386\O,0,0.970199
,0.495047,-0.340572\O,0,0.995901,-0.61238,-2.763399\O,0,-0.245701,-1.6
73391,-0.658898\C,0,-1.18756,2.298214,-0.268917\C,0,-1.785186,1.189899
,-0.875556\C,0,-3.123704,0.768258,-0.593491\C,0,-3.840443,1.481657,0.3
5866\H,0,-4.87257,1.193495,0.584258\C,0,-3.258698,2.562865,1.081292\C,
0,-1.904971,2.967818,0.789167\C,0,-1.314567,3.983284,1.60116\H,0,-0.27
3785,4.269614,1.425038\C,0,-2.032821,4.593562,2.618932\H,0,-1.553443,5
.362087,3.235233\C,0,-3.380332,4.224512,2.87466\H,0,-3.937023,4.715295
,3.680244\C,0,-3.976276,3.225593,2.122356\H,0,-5.003307,2.907269,2.332
214\C,0,0.178679,2.73197,-0.679857\C,0,1.23408,1.8163,-0.640458\C,0,2.
6038,2.19196,-0.803646\C,0,2.879591,3.512749,-1.126971\H,0,3.919351,3.
836141,-1.240988\C,0,1.838866,4.468232,-1.319241\C,0,0.466386,4.081804
,-1.097963\C,0,-0.554742,5.052041,-1.331083\H,0,-1.602281,4.763357,-1.
204111\C,0,-0.238509,6.341478,-1.73329\H,0,-1.040563,7.065612,-1.91399
\C,0,1.115485,6.728845,-1.920248\H,0,1.35254,7.751828,-2.232273\C,0,2.
130624,5.806131,-1.722216\H,0,3.178351,6.087305,-1.879013\C,0,-1.85464
6,-0.475044,4.129338\C,0,-1.433846,-1.670158,4.733017\H,0,-1.921972,-2
.02939,5.642599\C,0,-0.385379,-2.401096,4.164335\H,0,-0.065093,-3.3330
61,4.637908\C,0,0.220679,-1.961984,2.966241\C,0,-0.204243,-0.75043,2.3
75517\H,0,0.281395,-0.368611,1.475103\C,0,-1.23043,-0.008632,2.959284\
H,0,-1.546536,0.931794,2.500323\C,0,1.302314,-2.768354,2.358973\C,0,2.
262913,-3.494661,3.2496\H,0,3.231634,-3.650095,2.749523\H,0,1.855171,-
4.485127,3.523519\H,0,2.408149,-2.925043,4.180033\N,0,1.396878,-2.7985
36,1.051876\H,0,0.68173,-2.255608,0.435964\C,0,2.335528,-3.526719,0.25
4158\C,0,2.932618,-2.853057,-0.827604\H,0,2.734265,-1.792258,-0.999415
\C,0,3.808592,-3.550261,-1.668289\H,0,4.280286,-3.021967,-2.501798\C,0
,4.08446,-4.907183,-1.439404\C,0,3.47409,-5.574561,-0.365335\H,0,3.673
115,-6.636948,-0.190578\C,0,2.592053,-4.892033,0.482079\H,0,2.084234,-
5.421075,1.292372\C,0,3.677126,1.178141,-0.541044\C,0,4.395511,0.58249
5,-1.60878\C,0,3.954318,0.804129,0.805926\C,0,5.38773,-0.372519,-1.307
433\C,0,4.944978,-0.160564,1.051051\C,0,5.669797,-0.768155,0.00879\H,0
,5.943929,-0.841264,-2.127337\H,0,5.159782,-0.449526,2.084509\C,0,-3.7
12934,-0.396096,-1.329875\C,0,-4.021046,-1.603069,-0.641149\C,0,-3.963
894,-0.295761,-2.726614\C,0,-4.581217,-2.67338,-1.361811\C,0,-4.52359,
-1.397527,-3.399943\C,0,-4.838612,-2.596883,-2.741231\H,0,-4.814493,-3
.600796,-0.826029\H,0,-4.724026,-1.319488,-4.475684\H,0,4.770459,-5.44
6367,-2.101029\C,0,-2.996585,0.326635,4.704352\C,0,-3.687326,0.986128,
-3.515415\H,0,-3.217978,1.712849,-2.831449\C,0,-3.751628,-1.791627,0.8
5338\C,0,-5.426006,-3.781098,-3.504217\H,0,-5.554897,-3.458339,-4.5546
11\C,0,-5.068406,-1.881847,1.651256\H,0,-4.863912,-1.984342,2.731858\H
,0,-5.68708,-0.978615,1.505494\H,0,-5.666533,-2.756595,1.334575\C,0,-6
.813633,-4.181439,-2.963568\H,0,-6.748736,-4.536727,-1.918532\H,0,-7.5
14692,-3.32789,-2.989164\H,0,-7.246189,-4.998617,-3.569498\C,0,-4.4613
78,-4.985638,-3.499897\H,0,-4.871203,-5.815648,-4.104477\H,0,-3.476335
,-4.710393,-3.91711\H,0,-4.300932,-5.363294,-2.473053\C,0,-2.702368,0.
752166,-4.679038\H,0,-3.12654,0.070756,-5.43941\H,0,-2.471641,1.709514
,-5.181764\H,0,-1.756114,0.321113,-4.311801\C,0,-5.003231,1.622153,-4.
011796\H,0,-4.80084,2.577756,-4.530009\H,0,-5.528873,0.95805,-4.722511
\H,0,-5.688327,1.828242,-3.169577\C,0,6.738523,-1.818924,0.298118\H,0,
6.995168,-2.291614,-0.668758\C,0,4.119501,0.962683,-3.064479\H,0,3.139
59,1.469768,-3.08672\C,0,3.227662,1.478181,1.973222\H,0,2.198678,1.700
782,1.63969\C,0,8.019502,-1.160714,0.853573\H,0,8.811091,-1.915358,1.0
16186\H,0,8.4103,-0.397745,0.156779\H,0,7.818667,-0.664428,1.821308\C,
0,6.233466,-2.929215,1.241344\H,0,6.016294,-2.535015,2.250892\H,0,5.31
3501,-3.397323,0.850277\H,0,6.998843,-3.718762,1.35195\C,0,3.114002,0.
595803,3.228194\H,0,2.721159,-0.404985,2.983961\H,0,4.089184,0.464842,
3.731898\H,0,2.427137,1.062025,3.956608\C,0,3.898165,2.826202,2.321067
\H,0,3.926636,3.499374,1.446843\H,0,3.345556,3.338899,3.129944\H,0,4.9
37598,2.666139,2.662268\C,0,5.183624,1.955666,-3.578892\H,0,5.228303,2
.863971,-2.952747\H,0,6.188315,1.493042,-3.573123\H,0,4.957409,2.26578

4,-4.615768\C,0,4.010091,-0.259601,-3.995371\H,0,3.732366,0.069049,-5.
013843\H,0,4.96732,-0.806559,-4.078072\H,0,3.225816,-0.945552,-3.63722
1\C,0,-2.848787,-3.0126,1.124501\H,0,-3.345342,-3.959161,0.841396\H,0,
-1.907168,-2.926823,0.557512\H,0,-2.605256,-3.074171,2.200685\H,0,-3.2
07155,-0.903912,1.213586\F,0,-2.628395,1.60436,4.984289\F,0,-3.493028,
-0.205476,5.845489\F,0,-4.034666,0.412252,3.823795\\Version=ES64L-G09R
evD.01\State=1-A\HF=-3513.6185302\RMSD=1.979e-09\Dipole=2.4812717,-3.1
217463,4.4842739\Quadrupole=-8.3960565,20.8546422,-12.4585856,-15.9093
918,7.5129681,-20.8432461\PG=C01 [X(C65H69F3N1O4P1)]\\@

Conf2

1\1\GINC-WORKER2\SP\RTPSSTPSS\def2SVP\C65H69F3N1O4P1\JHIOE\07-May-2019
\0\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(sm
d,solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,0.24
8848,-0.6155,-1.398916\O,0,-0.979716,0.398412,-1.907559\O,0,0.999978,0
.402265,-0.26567\O,0,1.104995,-0.875547,-2.602143\O,0,-0.305698,-1.719
652,-0.501274\C,0,-1.108829,2.273267,-0.426609\C,0,-1.706501,1.152367,
-1.009425\C,0,-3.075015,0.792397,-0.795595\C,0,-3.827242,1.589129,0.05
7572\H,0,-4.882976,1.350768,0.224584\C,0,-3.25543,2.691786,0.754941\C,
0,-1.869898,3.031296,0.537186\C,0,-1.30077,4.076854,1.326119\H,0,-0.24
0739,4.319125,1.208238\C,0,-2.065499,4.773318,2.250593\H,0,-1.601898,5
.563441,2.851506\C,0,-3.440275,4.465482,2.431368\H,0,-4.032738,5.02353
3,3.164389\C,0,-4.018901,3.441344,1.699693\H,0,-5.068988,3.170008,1.85
4153\C,0,0.294111,2.638156,-0.776978\C,0,1.318084,1.696395,-0.627258\C
,0,2.703353,2.028231,-0.740742\C,0,3.032524,3.322775,-1.120036\H,0,4.0
86313,3.610948,-1.193654\C,0,2.033524,4.291262,-1.42588\C,0,0.641439,3
.951827,-1.26008\C,0,-0.338077,4.928383,-1.614387\H,0,-1.398773,4.6742
96,-1.53053\C,0,0.035532,6.181512,-2.077383\H,0,-0.735152,6.910297,-2.
351776\C,0,1.408027,6.525367,-2.206617\H,0,1.689964,7.520847,-2.566607
\C,0,2.384767,5.594463,-1.890517\H,0,3.447038,5.840607,-2.00098\C,0,-2
.169444,-0.153943,4.113601\C,0,-1.849614,-1.32973,4.810084\H,0,-2.4119
16,-1.610114,5.704465\C,0,-0.806938,-2.142893,4.353564\H,0,-0.568987,-
3.06172,4.896682\C,0,-0.102929,-1.80344,3.176944\C,0,-0.425747,-0.6085
13,2.493256\H,0,0.134591,-0.303409,1.606473\C,0,-1.449254,0.213336,2.9
63483\H,0,-1.688118,1.13909,2.432858\C,0,0.969944,-2.693104,2.682642\C
,0,1.810169,-3.452907,3.660895\H,0,2.786416,-3.720564,3.228535\H,0,1.2
96972,-4.387556,3.953602\H,0,1.953831,-2.852599,4.572306\N,0,1.166964,
-2.762127,1.389375\H,0,0.518714,-2.222582,0.699369\C,0,2.125687,-3.553
082,0.679704\C,0,2.867468,-2.916209,-0.332845\H,0,2.771181,-1.839402,-
0.495931\C,0,3.748358,-3.674368,-1.112456\H,0,4.331117,-3.178094,-1.89
3445\C,0,3.88748,-5.053557,-0.889771\C,0,3.139558,-5.680366,0.119151\H
,0,3.234965,-6.757897,0.288984\C,0,2.249445,-4.936183,0.905379\H,0,1.6
3284,-5.427553,1.662815\C,0,3.765467,1.032944,-0.377182\C,0,4.564284,0
.424773,-1.381264\C,0,4.007002,0.748641,0.995947\C,0,5.630305,-0.40922
9,-0.990961\C,0,5.083037,-0.091916,1.332939\C,0,5.921845,-0.663775,0.3
60139\H,0,6.255375,-0.863993,-1.767802\H,0,5.293241,-0.297839,2.388413
\C,0,-3.659712,-0.401406,-1.485848\C,0,-4.066686,-1.537694,-0.730557\C
,0,-3.8144,-0.400707,-2.899651\C,0,-4.630077,-2.635983,-1.405078\C,0,-
4.377112,-1.528735,-3.52542\C,0,-4.792863,-2.657328,-2.800713\H,0,-4.9
42846,-3.507929,-0.818744\H,0,-4.502544,-1.52682,-4.615222\H,0,4.57787
4,-5.640133,-1.50485\C,0,-3.307545,0.729424,4.562902\C,0,-3.433928,0.8
05695,-3.76088\H,0,-2.97439,1.561941,-3.103102\C,0,-3.893868,-1.624933
,0.787291\C,0,-5.401504,-3.865277,-3.507708\H,0,-5.397743,-3.641903,-4
.591193\C,0,-5.256188,-1.617021,1.509855\H,0,-5.116914,-1.660611,2.604
648\H,0,-5.829904,-0.702637,1.275747\H,0,-5.869913,-2.48735,1.211699\C
,0,-6.866906,-4.092791,-3.081474\H,0,-6.935754,-4.334549,-2.004674\H,0
,-7.481808,-3.193972,-3.267206\H,0,-7.311192,-4.934186,-3.64454\C,0,-4
.557315,-5.13787,-3.288351\H,0,-4.976098,-5.986334,-3.860117\H,0,-3.51
2883,-4.985899,-3.614097\H,0,-4.540827,-5.426935,-2.221281\C,0,-2.3931
84,0.443342,-4.839381\H,0,-2.803877,-0.271953,-5.575759\H,0,-2.082852,
1.349223,-5.392287\H,0,-1.494764,-0.003116,-4.381565\C,0,-4.687711,1.4
56049,-4.38328\H,0,-4.411961,2.361246,-4.95521\H,0,-5.199917,0.762556,
-5.075541\H,0,-5.410897,1.752604,-3.602242\C,0,7.109854,-1.528895,0.77
6893\H,0,7.182684,-1.461566,1.878883\C,0,4.305041,0.678184,-2.86776\H,
0,3.319659,1.168476,-2.948203\C,0,3.163294,1.396587,2.097355\H,0,2.154
281,1.564839,1.683746\C,0,6.895238,-3.01307,0.417973\H,0,7.747525,-3.6
24657,0.767489\H,0,5.975894,-3.407468,0.884225\H,0,6.807543,-3.149877,
-0.675099\C,0,8.434137,-1.002244,0.188969\H,0,8.441177,-1.074068,-0.91
4159\H,0,8.60005,0.055655,0.461031\H,0,9.289193,-1.591758,0.567436\C,0
,2.994728,0.510022,3.344079\H,0,2.666748,-0.50725,3.071494\H,0,3.93367
3,0.421141,3.920129\H,0,2.234758,0.944575,4.017576\C,0,3.735356,2.7777
98,2.484207\H,0,3.790411,3.448525,1.609064\H,0,3.098236,3.262203,3.246
995\H,0,4.754408,2.675193,2.900902\C,0,5.364675,1.634076,-3.455026\H,0
,5.390304,2.593137,-2.908529\H,0,6.374428,1.186341,-3.397803\H,0,5.148
166,1.850939,-4.517348\C,0,4.220822,-0.625855,-3.684132\H,0,3.978858,-
0.393235,-4.737593\H,0,5.177651,-1.179557,-3.680524\H,0,3.421334,-1.27
3975,-3.290858\C,0,-3.052607,-2.851372,1.195702\H,0,-3.571846,-3.79909

2,0.961327\H,0,-2.08375,-2.842064,0.670144\H,0,-2.862149,-2.83585,2.28
4116\H,0,-3.339262,-0.731706,1.117092\F,0,-3.872152,0.312726,5.71991\F
,0,-4.30122,0.770054,3.629369\F,0,-2.907349,2.013807,4.751115\\Version
=ES64L-G09RevD.01\State=1-A\HF=-3513.6167474\RMSD=1.969e-09\Dipole=1.9
921558,-2.8442456,4.8715654\Quadrupole=-9.8969745,17.7955698,-7.898595
3,-11.2991198,7.173432,-24.6882764\PG=C01 [X(C65H69F3N1O4P1)]\\@

Conf3

1\1\GINC-LOGIN\SP\RTPSSTPSS\def2SVP\C65H69F3N1O4P1\JHIOE\07-May-2019\0
\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(smd,
solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,0.2416
6,-0.738169,-1.28005\O,0,-1.016607,0.223816,-1.816845\O,0,1.012822,0.3
57843,-0.237022\O,0,1.06476,-1.066331,-2.489337\O,0,-0.271828,-1.79001
5,-0.298764\C,0,-1.144366,2.178335,-0.441213\C,0,-1.737875,1.021229,-0
.953116\C,0,-3.103587,0.668386,-0.710872\C,0,-3.853961,1.506031,0.1039
37\H,0,-4.908292,1.273857,0.287463\C,0,-3.282386,2.64664,0.737823\C,0,
-1.900509,2.980031,0.49075\C,0,-1.328512,4.066552,1.219881\H,0,-0.2701
32,4.305017,1.080939\C,0,-2.088273,4.807195,2.113544\H,0,-1.622683,5.6
28337,2.669644\C,0,-3.460728,4.505204,2.32018\H,0,-4.049834,5.099196,3
.027241\C,0,-4.041524,3.442556,1.647423\H,0,-5.089409,3.176744,1.82432
1\C,0,0.242558,2.549433,-0.843087\C,0,1.290614,1.6368,-0.678356\C,0,2.
663609,1.991897,-0.853644\C,0,2.952694,3.277711,-1.291425\H,0,3.997355
,3.584706,-1.406508\C,0,1.924948,4.211028,-1.609575\C,0,0.546313,3.846
27,-1.396981\C,0,-0.464605,4.780868,-1.775951\H,0,-1.516762,4.504411,-
1.661552\C,0,-0.131967,6.021375,-2.300063\H,0,-0.926264,6.71728,-2.591
894\C,0,1.228557,6.394026,-2.469873\H,0,1.477887,7.379886,-2.877331\C,
0,2.234562,5.501833,-2.134588\H,0,3.287882,5.768204,-2.278575\C,0,-2.2
09259,-0.038367,4.183184\C,0,-1.862898,-1.167958,4.940417\H,0,-2.43151
2,-1.426038,5.837513\C,0,-0.785417,-1.96518,4.540201\H,0,-0.526375,-2.
848623,5.130286\C,0,-0.072377,-1.657631,3.36041\C,0,-0.423347,-0.50925
2,2.613696\H,0,0.139591,-0.231239,1.719441\C,0,-1.481545,0.298315,3.02
8443\H,0,-1.743057,1.188243,2.449832\C,0,1.036413,-2.533648,2.925129\C
,0,1.895182,-3.204966,3.950623\H,0,2.882725,-3.465274,3.540212\H,0,1.4
09203,-4.137048,4.294214\H,0,2.011309,-2.546965,4.825457\N,0,1.24339,-
2.668649,1.638871\H,0,0.576537,-2.193567,0.919137\C,0,2.232276,-3.4624
21,0.976155\C,0,2.947568,-2.85781,-0.07484\H,0,2.80911,-1.7968,-0.3001
8\C,0,3.855694,-3.625873,-0.812226\H,0,4.415654,-3.154505,-1.624646\C,
0,4.049619,-4.982883,-0.508245\C,0,3.328463,-5.577558,0.538846\H,0,3.4
66584,-6.638529,0.771829\C,0,2.410418,-4.823813,1.282807\H,0,1.814596,
-5.294328,2.069545\C,0,3.768876,1.040709,-0.499623\C,0,4.530168,0.4081
71,-1.51812\C,0,4.099866,0.837777,0.868118\C,0,5.65483,-0.355383,-1.15
0667\C,0,5.233004,0.065579,1.183057\C,0,6.040214,-0.518464,0.19143\H,0
,6.252219,-0.827816,-1.938824\H,0,5.512632,-0.07421,2.233492\C,0,-3.69
3176,-0.55245,-1.34817\C,0,-4.09868,-1.656352,-0.549469\C,0,-3.860104,
-0.602548,-2.762035\C,0,-4.673764,-2.776697,-1.181521\C,0,-4.43362,-1.
746546,-3.342218\C,0,-4.852562,-2.846025,-2.571417\H,0,-4.987947,-3.63
0182,-0.56794\H,0,-4.566258,-1.775448,-4.430152\H,0,4.761927,-5.577226
,-1.089955\C,0,-3.37998,0.830048,4.574186\C,0,-3.482485,0.570271,-3.66
9909\H,0,-3.018831,1.350703,-3.044239\C,0,-3.912421,-1.68865,0.968738\
C,0,-5.475252,-4.078883,-3.220764\H,0,-5.748261,-4.770793,-2.401732\C,
0,-5.267802,-1.685436,1.704272\H,0,-5.117338,-1.68941,2.798488\H,0,-5.
862972,-0.791687,1.445409\H,0,-5.865974,-2.577907,1.442465\C,0,-4.4660
96,-4.806443,-4.1333\H,0,-4.162333,-4.165031,-4.981126\H,0,-3.554311,-
5.087428,-3.576699\H,0,-4.911812,-5.72828,-4.55049\C,0,-6.766643,-3.73
1412,-3.989471\H,0,-7.237197,-4.646918,-4.392913\H,0,-7.5004,-3.229699
,-3.333405\H,0,-6.556493,-3.058811,-4.841412\C,0,-2.447878,0.166097,-4
.73924\H,0,-2.862276,-0.577963,-5.444534\H,0,-2.141683,1.049948,-5.328
962\H,0,-1.546587,-0.261603,-4.269369\C,0,-4.738967,1.198386,-4.309056
\H,0,-4.465741,2.082064,-4.914883\H,0,-5.255658,0.480766,-4.972833\H,0
,-5.457607,1.523673,-3.53528\C,0,7.298644,-1.295186,0.573135\H,0,7.414
847,-1.198151,1.669117\C,0,4.164457,0.558984,-2.996249\H,0,3.147915,0.
986535,-3.038982\C,0,3.284257,1.49624,1.983397\H,0,2.262191,1.650344,1
.597399\C,0,7.171951,-2.797805,0.252526\H,0,8.082748,-3.339621,0.56764
8\H,0,6.308413,-3.245335,0.773821\H,0,7.038323,-2.965336,-0.831826\C,0
,8.557426,-0.693443,-0.084072\H,0,8.519168,-0.787057,-1.184998\H,0,8.6
64078,0.378417,0.161568\H,0,9.465797,-1.217913,0.265085\C,0,3.159442,0
.620502,3.2435\H,0,2.833078,-0.401716,2.986772\H,0,4.115609,0.542922,3
.792208\H,0,2.41657,1.054577,3.93625\C,0,3.856077,2.887034,2.332166\H,
0,3.883398,3.541888,1.443427\H,0,3.236295,3.381074,3.10303\H,0,4.88675
1,2.799263,2.72298\C,0,5.124822,1.53447,-3.707946\H,0,5.127716,2.52538
6,-3.221196\H,0,6.161215,1.148277,-3.694122\H,0,4.826982,1.672945,-4.7
63679\C,0,4.108728,-0.795852,-3.727838\H,0,3.787281,-0.644667,-4.77477
3\H,0,5.095942,-1.292607,-3.754728\H,0,3.37732,-1.463515,-3.245132\C,0
,-3.039505,-2.881729,1.40903\H,0,-3.539636,-3.847811,1.210894\H,0,-2.0
75469,-2.868726,0.874425\H,0,-2.839319,-2.825394,2.494575\H,0,-3.37452
5,-0.772929,1.26227\F,0,-3.989234,0.413059,5.708342\F,0,-4.331515,0.84
8725,3.597733\F,0,-3.007782,2.122007,4.770558\\Version=ES64L-G09RevD.0

1\State=1-A\HF=-3513.6166304\RMSD=1.907e-09\Dipole=2.1122496,-2.446963
7,5.0205169\Quadrupole=-9.3047597,13.4565063,-4.1517467,-11.6322936,8.
7764639,-26.6297609\PG=C01 [X(C65H69F3N1O4P1)]\\@

TRIP/2E Type II

Conf0

1\1\GINC-WORKER0\SP\RTPSSTPSS\def2SVP\C65H69F3N1O4P1\JHIOE\05-May-2019
\0\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(sm
d,solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,-0.2
51952,-0.545172,-0.840162\O,0,-1.686442,0.133539,-1.371612\O,0,0.39618
4,0.802852,-0.02757\O,0,0.524169,-0.918084,-2.066325\O,0,-0.512652,-1.
506699,0.316919\C,0,-2.083801,2.125352,-0.109826\C,0,-2.467103,0.83149
8,-0.471335\C,0,-3.670434,0.210293,-0.013452\C,0,-4.472848,0.927311,0.
863281\H,0,-5.416291,0.492632,1.208529\C,0,-4.091737,2.21078,1.350367\
C,0,-2.872426,2.819863,0.877657\C,0,-2.472397,4.063822,1.453238\H,0,-1
.52827,4.51782,1.139665\C,0,-3.249096,4.689401,2.41799\H,0,-2.913883,5
.637663,2.852269\C,0,-4.469538,4.106599,2.853337\H,0,-5.076122,4.61328
2,3.611815\C,0,-4.877781,2.889836,2.329695\H,0,-5.804779,2.417418,2.67
4142\C,0,-0.859525,2.727994,-0.711635\C,0,0.361696,2.0518,-0.617078\C,
0,1.606158,2.633806,-1.014384\C,0,1.578032,3.891831,-1.600916\H,0,2.51
7839,4.368235,-1.899021\C,0,0.353933,4.581169,-1.83898\C,0,-0.88807,3.
997164,-1.394972\C,0,-2.101982,4.692299,-1.682225\H,0,-3.055235,4.2448
16,-1.386108\C,0,-2.088941,5.912479,-2.341871\H,0,-3.033926,6.423533,-
2.556818\C,0,-0.861701,6.501512,-2.748755\H,0,-0.86486,7.468094,-3.264
226\C,0,0.333522,5.843784,-2.504671\H,0,1.28588,6.279069,-2.828444\C,0
,4.070366,-3.376393,-0.249454\C,0,4.0378,-4.088876,0.964138\H,0,4.6162
57,-5.010441,1.077557\C,0,3.265427,-3.613435,2.026168\H,0,3.233772,-4.
174672,2.964424\C,0,2.507507,-2.42816,1.877132\C,0,2.566129,-1.715677,
0.661156\H,0,2.064251,-0.751068,0.561529\C,0,3.334336,-2.193702,-0.402
201\H,0,3.367777,-1.631715,-1.335922\C,0,1.695372,-1.908959,2.998581\C
,0,2.237219,-1.99344,4.390535\H,0,1.821551,-1.205811,5.037672\H,0,3.33
4955,-1.918173,4.364184\H,0,1.977738,-2.972671,4.834624\N,0,0.549062,-
1.343593,2.70497\H,0,0.19816,-1.372517,1.671547\C,0,-0.376241,-0.69317
6,3.577985\C,0,-0.934058,0.513627,3.11298\H,0,-0.630648,0.907413,2.138
692\C,0,-1.864264,1.190537,3.910151\H,0,-2.285127,2.136889,3.558827\C,
0,-2.261834,0.653957,5.145178\C,0,-1.72626,-0.566991,5.584764\H,0,-2.0
51796,-1.001034,6.53581\C,0,-0.780856,-1.248603,4.806012\H,0,-0.394026
,-2.216991,5.132053\C,0,2.896947,1.922099,-0.739085\C,0,3.631145,1.318
277,-1.792018\C,0,3.390329,1.872093,0.596059\C,0,4.855227,0.689278,-1.
488904\C,0,4.61569,1.231304,0.845078\C,0,5.363592,0.627377,-0.182537\H
,0,5.422647,0.210529,-2.296117\H,0,4.995691,1.195708,1.870811\C,0,-4.0
58719,-1.150209,-0.508425\C,0,-4.026703,-2.271901,0.364245\C,0,-4.4792
54,-1.313049,-1.858056\C,0,-4.465015,-3.51933,-0.121424\C,0,-4.89411,-
2.582789,-2.296022\C,0,-4.903596,-3.700043,-1.44274\H,0,-4.45097,-4.38
7164,0.548438\H,0,-5.219111,-2.70154,-3.336389\H,0,-2.999244,1.182388,
5.758386\C,0,4.995207,-3.828013,-1.351502\C,0,-4.505466,-0.147924,-2.8
49377\H,0,-4.148374,0.75401,-2.3246\C,0,-3.516566,-2.168645,1.803758\C
,0,-5.349586,-5.072379,-1.93917\H,0,-5.301435,-5.760815,-1.074433\C,0,
-4.679989,-2.130262,2.816915\H,0,-4.293638,-2.020162,3.846978\H,0,-5.3
65704,-1.288452,2.619205\H,0,-5.270276,-3.064698,2.772086\C,0,-4.39281
5,-5.613453,-3.022\H,0,-4.409526,-4.973593,-3.92363\H,0,-3.352561,-5.6
49988,-2.652098\H,0,-4.686039,-6.634725,-3.3277\C,0,-6.806377,-5.05551
4,-2.444013\H,0,-7.126749,-6.070352,-2.743539\H,0,-7.496729,-4.694917,
-1.660387\H,0,-6.916907,-4.395413,-3.324098\C,0,-3.550195,-0.396414,-4
.035022\H,0,-3.875478,-1.262501,-4.640774\H,0,-3.524507,0.486835,-4.69
987\H,0,-2.525095,-0.587201,-3.675514\C,0,-5.939347,0.151845,-3.332855
\H,0,-5.944334,1.026589,-4.009004\H,0,-6.366957,-0.703937,-3.887066\H,
0,-6.60888,0.374066,-2.482419\C,0,6.690886,-0.072664,0.097563\H,0,6.90
5791,-0.709395,-0.780595\C,0,3.138801,1.34194,-3.24045\H,0,2.090887,1.
688379,-3.228374\C,0,2.628759,2.547519,1.739311\H,0,1.556707,2.527806,
1.479409\C,0,7.836441,0.953886,0.2257\H,0,8.804933,0.444331,0.384216\H
,0,7.92009,1.573873,-0.68473\H,0,7.662188,1.63068,1.082848\C,0,6.63040
6,-0.991765,1.332753\H,0,6.511514,-0.411484,2.266048\H,0,5.788852,-1.7
01747,1.263008\H,0,7.563887,-1.57615,1.422711\C,0,2.775196,1.824095,3.
089284\H,0,2.550374,0.748668,2.992472\H,0,3.794658,1.921889,3.504622\H
,0,2.076217,2.254437,3.828207\C,0,3.042245,4.030214,1.862013\H,0,2.876
749,4.570615,0.913377\H,0,2.455801,4.535125,2.651788\H,0,4.113753,4.11
6506,2.120907\C,0,3.960282,2.348706,-4.073364\H,0,3.916668,3.362742,-3
.637623\H,0,5.023164,2.046532,-4.120566\H,0,3.576208,2.40442,-5.108578
\C,0,3.140843,-0.056214,-3.88981\H,0,2.760996,0.00966,-4.926259\H,0,4.
155696,-0.491277,-3.937157\H,0,2.480238,-0.73615,-3.328034\C,0,-2.5335
52,-3.303975,2.153525\H,0,-3.035274,-4.288621,2.176648\H,0,-1.708758,-
3.34065,1.423742\H,0,-2.10222,-3.133213,3.155677\H,0,-2.959905,-1.2199
7,1.886103\F,0,6.283339,-3.447421,-1.101036\F,0,5.01629,-5.177441,-1.4
8729\F,0,4.665221,-3.304462,-2.556418\\Version=ES64L-G09RevD.01\State=

1-A\HF=-3513.6179709\RMSD=2.124e-09\Dipole=0.8325238,-0.1111922,6.2971
94\Quadrupole=-12.1824579,-1.5461594,13.7286173,-8.0052176,9.0546708,-
21.7894102\PG=C01 [X(C65H69F3N1O4P1)]\\@

Conf1

1\1\GINC-WORKER1\SP\RTPSSTPSS\def2SVP\C65H69F3N1O4P1\JHIOE\29-Apr-2019
\0\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(sm
d,solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,-0.2
48114,-0.485061,-0.9228\O,0,-1.651579,0.261392,-1.44765\O,0,0.419767,0
.796826,-0.023022\O,0,0.545179,-0.815673,-2.150073\O,0,-0.562253,-1.49
8432,0.175229\C,0,-2.025525,2.184446,-0.077923\C,0,-2.433915,0.92503,-
0.522562\C,0,-3.661407,0.310096,-0.124352\C,0,-4.459601,0.99269,0.7830
82\H,0,-5.419562,0.562791,1.08644\C,0,-4.055121,2.234104,1.353276\C,0,
-2.814045,2.839889,0.936139\C,0,-2.394694,4.037855,1.590129\H,0,-1.435
448,4.487016,1.318072\C,0,-3.172288,4.623771,2.578893\H,0,-2.822402,5.
536228,3.074023\C,0,-4.412957,4.046079,2.960605\H,0,-5.019915,4.521784
,3.738567\C,0,-4.840967,2.872825,2.35934\H,0,-5.784435,2.403772,2.6607
25\C,0,-0.774106,2.78886,-0.618733\C,0,0.429152,2.080385,-0.532645\C,0
,1.696649,2.660497,-0.852918\C,0,1.711256,3.952277,-1.362034\H,0,2.669
695,4.425915,-1.599907\C,0,0.508527,4.678543,-1.599224\C,0,-0.75761,4.
093893,-1.230883\C,0,-1.949393,4.826423,-1.517463\H,0,-2.919319,4.3811
84,-1.277\C,0,-1.893671,6.079358,-2.110258\H,0,-2.822193,6.618326,-2.3
28605\C,0,-0.643564,6.666949,-2.443037\H,0,-0.613372,7.659375,-2.90587
5\C,0,0.531856,5.975579,-2.195271\H,0,1.501803,6.410474,-2.46244\C,0,3
.985104,-3.40304,-0.417265\C,0,3.896421,-4.214082,0.729855\H,0,4.44551
,-5.158843,0.780385\C,0,3.106534,-3.806527,1.807553\H,0,3.031344,-4.44
3031,2.693917\C,0,2.386864,-2.590983,1.738594\C,0,2.500526,-1.780966,0
.589391\H,0,2.026158,-0.798113,0.557683\C,0,3.287073,-2.189765,-0.4888
85\H,0,3.365246,-1.550558,-1.368737\C,0,1.55629,-2.139436,2.875442\C,0
,2.049474,-2.351017,4.271855\H,0,1.644612,-1.597523,4.965121\H,0,3.149
617,-2.322065,4.285122\H,0,1.734218,-3.348973,4.630671\N,0,0.435649,-1
.519203,2.593064\H,0,0.113746,-1.466883,1.550802\C,0,-0.493085,-0.8971
48,3.482715\C,0,-0.991991,0.358884,3.085757\H,0,-0.64619,0.804502,2.14
8485\C,0,-1.919143,1.017159,3.901714\H,0,-2.293734,2.000804,3.604371\C
,0,-2.372325,0.414992,5.086491\C,0,-1.895666,-0.852607,5.456235\H,0,-2
.265082,-1.336227,6.366437\C,0,-0.953764,-1.517397,4.658702\H,0,-0.612
101,-2.519509,4.928719\C,0,2.965433,1.910583,-0.57768\C,0,3.739383,1.3
76229,-1.639282\C,0,3.403227,1.76147,0.77036\C,0,4.943534,0.710932,-1.
331527\C,0,4.609845,1.087932,1.023082\C,0,5.394456,0.547925,-0.013259\
H,0,5.539806,0.283482,-2.146868\H,0,4.946706,0.975539,2.058304\C,0,-4.
080668,-1.002127,-0.715232\C,0,-4.087463,-2.183884,0.077835\C,0,-4.493
733,-1.057077,-2.073525\C,0,-4.553928,-3.380853,-0.494781\C,0,-4.93935
4,-2.283559,-2.601811\C,0,-4.986494,-3.455557,-1.830772\H,0,-4.56617,-
4.28862,0.118803\H,0,-5.261689,-2.327886,-3.649495\H,0,-3.106917,0.929
696,5.714591\C,0,4.931229,-3.781802,-1.528988\C,0,-4.482382,0.176679,-
2.97775\H,0,-4.111915,1.029402,-2.384281\C,0,-3.592384,-2.191387,1.526
215\C,0,-5.473762,-4.770546,-2.432735\H,0,-5.761376,-4.559934,-3.48009
3\C,0,-4.768568,-2.17539,2.524911\H,0,-4.395003,-2.144142,3.564942\H,0
,-5.421469,-1.299075,2.37148\H,0,-5.390106,-3.083459,2.412479\C,0,-6.7
23123,-5.304566,-1.702821\H,0,-6.495502,-5.552004,-0.649458\H,0,-7.537
219,-4.557732,-1.707789\H,0,-7.096609,-6.223527,-2.190873\C,0,-4.35162
2,-5.828612,-2.459822\H,0,-4.698064,-6.751857,-2.959759\H,0,-3.465104,
-5.454652,-3.002363\H,0,-4.033623,-6.098661,-1.435899\C,0,-3.517405,-0
.00556,-4.167376\H,0,-3.85454,-0.815539,-4.840456\H,0,-3.461505,0.9242
7,-4.763223\H,0,-2.502005,-0.24753,-3.810772\C,0,-5.90322,0.543866,-3.
45363\H,0,-5.880854,1.468561,-4.05924\H,0,-6.341202,-0.256719,-4.07772
3\H,0,-6.579043,0.714161,-2.596224\C,0,6.698298,-0.192356,0.273305\H,0
,6.960801,-0.743449,-0.648853\C,0,3.307154,1.498294,-3.102041\H,0,2.27
97,1.900996,-3.112625\C,0,2.60542,2.371917,1.925987\H,0,1.542214,2.370
606,1.631673\C,0,7.841893,0.800627,0.570144\H,0,8.795517,0.264318,0.73
0299\H,0,7.982474,1.50816,-0.266514\H,0,7.624878,1.389694,1.480666\C,0
,6.554523,-1.227113,1.406135\H,0,6.379981,-0.739057,2.382543\H,0,5.714
47,-1.915512,1.213516\H,0,7.476555,-1.829411,1.49696\C,0,2.707288,1.57
4262,3.237891\H,0,2.481695,0.506924,3.075749\H,0,3.713567,1.64448,3.68
9217\H,0,1.987189,1.967118,3.977329\C,0,3.017161,3.844113,2.145166\H,0
,2.881531,4.437246,1.223917\H,0,2.406818,4.306062,2.943029\H,0,4.08017
3,3.911813,2.441605\C,0,4.210558,2.495863,-3.85651\H,0,4.209748,3.4870
94,-3.368973\H,0,5.255926,2.136577,-3.89097\H,0,3.861769,2.625711,-4.8
97565\C,0,3.259251,0.131301,-3.814024\H,0,2.945072,0.264475,-4.865916\
H,0,4.245876,-0.366475,-3.823343\H,0,2.526193,-0.527782,-3.32076\C,0,-
2.655,-3.381299,1.814481\H,0,-3.193498,-4.346076,1.778996\H,0,-1.82738
8,-3.407692,1.087477\H,0,-2.22333,-3.284523,2.826397\H,0,-3.003684,-1.
270617,1.675258\F,0,6.213574,-3.416311,-1.23059\F,0,4.958105,-5.118841
,-1.753577\F,0,4.621834,-3.179848,-2.702842\\Version=ES64L-G09RevD.01\
State=1-A\HF=-3513.617892\RMSD=2.134e-09\Dipole=0.6465577,-0.5445866,6
.321251\Quadrupole=-12.7337149,2.208718,10.5249969,-7.6431537,7.197817
8,-22.9913322\PG=C01 [X(C65H69F3N1O4P1)]\\@

Conf2

1\1\GINC-WORKER0\SP\RTPSSTPSS\def2SVP\C65H69F3N1O4P1\JHIOE\05-May-2019
\0\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(sm
d,solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,-0.1
99774,-0.548596,-0.802434\O,0,-1.605893,0.13503,-1.402888\O,0,0.431112
,0.805965,0.011259\O,0,0.62044,-0.954142,-1.988707\O,0,-0.522552,-1.48
4675,0.360049\C,0,-2.027101,2.15611,-0.197761\C,0,-2.411105,0.858798,-
0.545394\C,0,-3.636843,0.260608,-0.116802\C,0,-4.463175,1.006342,0.712
521\H,0,-5.42443,0.590675,1.031037\C,0,-4.086752,2.297219,1.183457\C,0
,-2.843769,2.882003,0.743436\C,0,-2.452127,4.135441,1.304237\H,0,-1.49
1351,4.571713,1.017484\C,0,-3.258919,4.793118,2.221846\H,0,-2.93031,5.
748574,2.645263\C,0,-4.501808,4.233882,2.623257\H,0,-5.132121,4.765617
,3.344327\C,0,-4.90231,3.008149,2.114746\H,0,-5.84705,2.553776,2.43436
6\C,0,-0.772755,2.731555,-0.761896\C,0,0.435607,2.044438,-0.600159\C,0
,1.701992,2.608832,-0.947496\C,0,1.713564,3.859488,-1.551281\H,0,2.671
206,4.323751,-1.809351\C,0,0.509822,4.558071,-1.854282\C,0,-0.757255,3
.989934,-1.46476\C,0,-1.94934,4.692463,-1.817872\H,0,-2.91994,4.255771
,-1.565246\C,0,-1.892975,5.906151,-2.487\H,0,-2.821743,6.423193,-2.752
274\C,0,-0.641881,6.481315,-2.837595\H,0,-0.611013,7.443506,-3.360359\
C,0,0.533802,5.814438,-2.531622\H,0,1.505039,6.237642,-2.812478\C,0,3.
87503,-3.512219,-0.038626\C,0,3.695489,-4.262052,1.139613\H,0,4.158076
,-5.248537,1.241368\C,0,2.927122,-3.740854,2.182368\H,0,2.781766,-4.32
6622,3.094751\C,0,2.311627,-2.475475,2.042688\C,0,2.517391,-1.726477,0
.865627\H,0,2.115327,-0.714428,0.777278\C,0,3.294409,-2.244246,-0.1737
83\H,0,3.453249,-1.650442,-1.074817\C,0,1.488218,-1.917218,3.137643\C,
0,1.963929,-2.051658,4.548967\H,0,1.586481,-1.236289,5.185514\H,0,3.06
4184,-2.066009,4.568466\H,0,1.607829,-3.009145,4.973465\N,0,0.391474,-
1.284602,2.798018\H,0,0.090403,-1.308785,1.747074\C,0,-0.53786,-0.5855
64,3.626598\C,0,-1.036617,0.630109,3.118338\H,0,-0.68868,0.991709,2.14
636\C,0,-1.967352,1.357275,3.869186\H,0,-2.342822,2.309533,3.484086\C,
0,-2.424779,0.863081,5.101222\C,0,-1.948781,-0.366165,5.583538\H,0,-2.
321046,-0.767966,6.531576\C,0,-1.00387,-1.098395,4.85169\H,0,-0.666811
,-2.07278,5.212209\C,0,2.980165,1.905149,-0.601172\C,0,3.778714,1.3135
01,-1.615481\C,0,3.418151,1.888542,0.752563\C,0,5.023192,0.757885,-1.2
62063\C,0,4.669061,1.319426,1.05314\C,0,5.495639,0.763498,0.061066\H,0
,5.641631,0.308567,-2.047655\H,0,5.023486,1.318206,2.090105\C,0,-4.025
412,-1.105413,-0.596509\C,0,-4.021341,-2.212598,0.294787\C,0,-4.420427
,-1.286242,-1.951283\C,0,-4.461335,-3.463763,-0.179444\C,0,-4.83914,-2
.558962,-2.377006\C,0,-4.876331,-3.66185,-1.506017\H,0,-4.46942,-4.320
213,0.5049\H,0,-5.144982,-2.691616,-3.421512\H,0,-3.162697,1.430603,5.
677757\C,0,4.735202,-4.083088,-1.13898\C,0,-4.414298,-0.136095,-2.9598
47\H,0,-4.05668,0.76905,-2.441017\C,0,-3.543502,-2.087929,1.74326\C,0,
-5.326651,-5.037868,-1.987987\H,0,-5.298114,-5.712977,-1.111961\C,0,-4
.730216,-2.00278,2.726392\H,0,-4.366996,-1.878576,3.763232\H,0,-5.3926
74,-1.151323,2.494311\H,0,-5.339328,-2.925275,2.686396\C,0,-4.358385,-
5.605062,-3.04683\H,0,-4.356368,-4.981138,-3.959729\H,0,-3.324138,-5.6
43394,-2.66066\H,0,-4.655485,-6.629215,-3.338892\C,0,-6.775281,-5.0160
74,-2.515628\H,0,-7.100395,-6.032768,-2.803514\H,0,-7.474326,-4.636262
,-1.748952\H,0,-6.865952,-4.369662,-3.408096\C,0,-3.438757,-0.411768,-
4.122684\H,0,-3.760383,-1.283698,-4.721965\H,0,-3.391078,0.461278,-4.7
99659\H,0,-2.422901,-0.607425,-3.739706\C,0,-5.835763,0.172441,-3.4729
5\H,0,-5.819343,1.037,-4.16188\H,0,-6.263477,-0.686643,-4.021992\H,0,-
6.51661,0.41391,-2.636785\C,0,6.864018,0.186577,0.416452\H,0,7.012486,
0.351193,1.500425\C,0,3.334578,1.284179,-3.079673\H,0,2.28426,1.621223
,-3.114174\C,0,2.585453,2.541878,1.858711\H,0,1.529176,2.50719,1.54318
5\C,0,6.925975,-1.332279,0.158923\H,0,7.913447,-1.738312,0.445766\H,0,
6.155496,-1.867452,0.739196\H,0,6.764407,-1.56155,-0.909159\C,0,7.9978
38,0.920898,-0.328222\H,0,7.924165,0.765866,-1.420391\H,0,7.964537,2.0
08406,-0.13649\H,0,8.984891,0.545072,-0.001759\C,0,2.672991,1.808471,3
.209007\H,0,2.462963,0.731686,3.093726\H,0,3.669461,1.912895,3.675215\
H,0,1.934442,2.226315,3.916034\C,0,2.967832,4.02992,2.013394\H,0,2.843
057,4.574286,1.060714\H,0,2.332498,4.519715,2.774389\H,0,4.022654,4.13
162,2.328864\C,0,4.173095,2.266179,-3.924492\H,0,4.112469,3.294314,-3.
525122\H,0,5.238633,1.969945,-3.934325\H,0,3.815896,2.283561,-4.970579
\C,0,3.36873,-0.138461,-3.673478\H,0,3.038577,-0.114722,-4.728633\H,0,
4.38562,-0.570789,-3.653394\H,0,2.682607,-0.798294,-3.118255\C,0,-2.59
4175,-3.235098,2.143013\H,0,-3.11834,-4.207582,2.180857\H,0,-1.754612,
-3.309334,1.433285\H,0,-2.181037,-3.047375,3.149796\H,0,-2.968789,-1.1
49248,1.816951\F,0,5.983736,-4.390295,-0.689173\F,0,4.218331,-5.235774
,-1.640848\F,0,4.889151,-3.230379,-2.181083\\Version=ES64L-G09RevD.01\
State=1-A\HF=-3513.6172209\RMSD=2.115e-09\Dipole=0.5290941,0.0499115,6
.3688697\Quadrupole=-12.6365377,-2.7823625,15.4189002,-5.5071238,7.211
5688,-22.5331701\PG=C01 [X(C65H69F3N1O4P1)]\\@

Conf3

1\1\GINC-WORKER1\SP\RTPSSTPSS\def2SVP\C65H69F3N1O4P1\JHIOE\05-May-2019

\0\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(sm
d,solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,-0.1
80576,-0.486323,-0.860199\O,0,-1.551045,0.26135,-1.467754\O,0,0.458012
,0.808245,0.040932\O,0,0.666057,-0.853605,-2.0403\O,0,-0.563758,-1.470
239,0.242878\C,0,-1.966595,2.219387,-0.161168\C,0,-2.367637,0.953751,-
0.595075\C,0,-3.619649,0.362264,-0.240258\C,0,-4.454386,1.078329,0.606
624\H,0,-5.434563,0.668544,0.87057\C,0,-4.063849,2.329673,1.164711\C,0
,-2.795234,2.909012,0.796549\C,0,-2.392808,4.118203,1.440626\H,0,-1.41
4068,4.547023,1.207398\C,0,-3.212086,4.73988,2.372301\H,0,-2.875571,5.
660504,2.861508\C,0,-4.478752,4.187974,2.703907\H,0,-5.118478,4.691594
,3.43676\C,0,-4.891325,3.004307,2.112244\H,0,-5.855196,2.554807,2.3766
76\C,0,-0.685059,2.798111,-0.655946\C,0,0.504796,2.078775,-0.498161\C,
0,1.791099,2.636597,-0.776692\C,0,1.843095,3.91822,-1.30974\H,0,2.8165
5,4.376143,-1.514886\C,0,0.661673,4.654206,-1.612211\C,0,-0.626515,4.0
89695,-1.293012\C,0,-1.794995,4.830205,-1.647377\H,0,-2.780375,4.39960
8,-1.447143\C,0,-1.697187,6.072721,-2.256252\H,0,-2.608391,6.618021,-2
.52571\C,0,-0.426272,6.641251,-2.539926\H,0,-0.36306,7.625598,-3.01650
9\C,0,0.727976,5.940406,-2.228256\H,0,1.714512,6.359079,-2.457858\C,0,
3.774629,-3.544839,-0.175494\C,0,3.543991,-4.376084,0.937725\H,0,3.972
912,-5.382239,0.972327\C,0,2.764338,-3.912799,1.999535\H,0,2.578037,-4
.563024,2.859295\C,0,2.189021,-2.622127,1.94255\C,0,2.448818,-1.791997
,0.832529\H,0,2.075962,-0.765306,0.810381\C,0,3.237292,-2.252002,-0.22
5055\H,0,3.435134,-1.595316,-1.073167\C,0,1.342938,-2.121864,3.048961\
C,0,1.766338,-2.359538,4.463359\H,0,1.387299,-1.576383,5.138423\H,0,2.
864694,-2.404847,4.517205\H,0,1.371841,-3.332646,4.812067\N,0,0.271707
,-1.444086,2.715279\H,0,0.006541,-1.396369,1.655398\C,0,-0.671365,-0.7
75518,3.552856\C,0,-1.129046,0.476902,3.097622\H,0,-0.742249,0.883048,
2.158379\C,0,-2.068784,1.182139,3.857765\H,0,-2.412352,2.162061,3.5144
23\C,0,-2.576064,0.630707,5.045249\C,0,-2.141461,-0.633731,5.472693\H,
0,-2.553448,-1.079194,6.384108\C,0,-1.187899,-1.34541,4.731563\H,0,-0.
883178,-2.345591,5.04757\C,0,3.046763,1.888075,-0.442535\C,0,3.865024,
1.353119,-1.47258\C,0,3.447075,1.772284,0.918477\C,0,5.089809,0.752124
,-1.124309\C,0,4.679289,1.161028,1.213088\C,0,5.524859,0.659222,0.2080
34\H,0,5.722084,0.344792,-1.921663\H,0,5.004499,1.082852,2.256577\C,0,
-4.029437,-0.960231,-0.815649\C,0,-4.067244,-2.124247,0.002419\C,0,-4.
406805,-1.040691,-2.182637\C,0,-4.533571,-3.32825,-0.55517\C,0,-4.8565
7,-2.272928,-2.694249\C,0,-4.937825,-3.426424,-1.898744\H,0,-4.570117,
-4.22262,0.076787\H,0,-5.15266,-2.33716,-3.748656\H,0,-3.320785,1.1816
86,5.629046\C,0,4.636258,-4.059352,-1.302137\C,0,-4.34272,0.169678,-3.
115538\H,0,-3.978661,1.030525,-2.529803\C,0,-3.605204,-2.101368,1.4613
18\C,0,-5.427713,-4.748307,-2.483495\H,0,-5.696597,-4.554802,-3.539081
\C,0,-4.800309,-2.014758,2.43373\H,0,-4.446337,-1.966934,3.479992\H,0,
-5.41696,-1.119916,2.242859\H,0,-5.452832,-2.902286,2.333402\C,0,-6.69
3209,-5.258394,-1.764501\H,0,-6.484358,-5.490468,-0.703796\H,0,-7.5004
49,-4.504749,-1.794498\H,0,-7.067377,-6.182083,-2.243037\C,0,-4.314575
,-5.816423,-2.472255\H,0,-4.662024,-6.747121,-2.957474\H,0,-3.417027,-
5.461918,-3.009657\H,0,-4.013919,-6.066976,-1.438188\C,0,-3.336388,-0.
059596,-4.262368\H,0,-3.658332,-0.885585,-4.923282\H,0,-3.246275,0.851
478,-4.882494\H,0,-2.338371,-0.302791,-3.860187\C,0,-5.738134,0.549178
,-3.651827\H,0,-5.677331,1.458872,-4.277145\H,0,-6.167421,-0.258114,-4
.273331\H,0,-6.440988,0.750558,-2.823262\C,0,6.869034,0.026349,0.56019
9\H,0,7.010784,0.153128,1.650111\C,0,3.462475,1.422722,-2.947511\H,0,2
.425824,1.798468,-2.992756\C,0,2.595833,2.367643,2.043315\H,0,1.545475
,2.352766,1.707371\C,0,6.877447,-1.485808,0.258557\H,0,7.847019,-1.936
183,0.540385\H,0,6.082776,-2.008217,0.817669\H,0,6.715685,-1.676417,-0
.816944\C,0,8.038129,0.738051,-0.150268\H,0,7.974831,0.615926,-1.24720
7\H,0,8.042739,1.820383,0.071066\H,0,9.005913,0.31655,0.177771\C,0,2.6
57363,1.563723,3.35436\H,0,2.454138,0.493969,3.177542\H,0,3.64333,1.64
6002,3.846492\H,0,1.902554,1.941438,4.066781\C,0,2.978139,3.844424,2.2
83562\H,0,2.871043,4.438222,1.358832\H,0,2.329559,4.295375,3.057258\H,
0,4.027213,3.92648,2.62287\C,0,4.357704,2.418269,-3.714343\H,0,4.31963
1,3.425057,-3.261469\H,0,5.412578,2.086145,-3.71274\H,0,4.030812,2.504
244,-4.766908\C,0,3.465181,0.032983,-3.616393\H,0,3.172674,0.124098,-4
.678965\H,0,4.464516,-0.437872,-3.586033\H,0,2.7378,-0.62952,-3.119488
\C,0,-2.712603,-3.309066,1.809444\H,0,-3.279507,-4.258013,1.794062\H,0
,-1.870146,-3.385582,1.103297\H,0,-2.300514,-3.191687,2.82754\H,0,-2.9
89799,-1.195334,1.591762\F,0,5.861316,-4.454544,-0.856814\F,0,4.083811
,-5.143494,-1.907801\F,0,4.847391,-3.131227,-2.267282\\Version=ES64L-G
09RevD.01\State=1-A\HF=-3513.6171451\RMSD=2.061e-09\Dipole=0.3160675,-
0.3493171,6.3937597\Quadrupole=-12.9074242,0.2214301,12.6859941,-4.978
4625,5.5676663,-23.7363564\PG=C01 [X(C65H69F3N1O4P1)]\\@

TRIP/2E Switching TS

Conf0
1\1\GINC-WORKER0\SP\RTPSSTPSS\def2SVP\C65H69F3N1O4P1\JHIOE\29-Apr-2019

\0\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(sm
d,solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,-0.1
26727,0.039424,-0.427595\O,0,1.122372,0.953558,0.226313\O,0,-1.277575,
1.259786,-0.602067\O,0,-0.523336,-0.940285,0.656727\O,0,0.159356,-0.47
6635,-1.819212\C,0,0.564954,3.27472,-0.00941\C,0,1.425549,2.203494,-0.
269942\C,0,2.672104,2.352344,-0.955731\C,0,3.012038,3.615648,-1.42058\
H,0,3.969574,3.76342,-1.93125\C,0,2.128303,4.725661,-1.285174\C,0,0.87
6387,4.55797,-0.587492\C,0,-0.017267,5.669988,-0.526413\H,0,-0.986816,
5.547464,-0.03477\C,0,0.320205,6.891616,-1.090391\H,0,-0.386196,7.7274
71,-1.03726\C,0,1.569928,7.065418,-1.743638\H,0,1.827534,8.036832,-2.1
79786\C,0,2.451519,6.000296,-1.841048\H,0,3.409915,6.115752,-2.360217\
C,0,-0.637072,3.054098,0.843971\C,0,-1.538597,2.03931,0.509706\C,0,-2.
754296,1.804641,1.227332\C,0,-3.031488,2.621828,2.314477\H,0,-3.973926
,2.497224,2.857334\C,0,-2.113133,3.616156,2.7608\C,0,-0.884253,3.82769
3,2.035475\C,0,0.050818,4.774349,2.554\H,0,1.007519,4.913955,2.042514\
C,0,-0.229717,5.50355,3.700339\H,0,0.506933,6.218974,4.082351\C,0,-1.4
60052,5.325011,4.387956\H,0,-1.672511,5.911663,5.288449\C,0,-2.37836,4
.3946,3.92766\H,0,-3.321176,4.229625,4.461788\C,0,-3.707911,0.742521,0
.76457\C,0,-3.810459,-0.496282,1.457817\C,0,-4.513469,0.9871,-0.378677
\C,0,-4.717653,-1.461167,0.983817\C,0,-5.409687,-0.010176,-0.808611\C,
0,-5.523754,-1.243845,-0.148223\H,0,-4.79679,-2.415575,1.51574\H,0,-6.
032754,0.176304,-1.691891\C,0,3.561415,1.160903,-1.139782\C,0,3.756959
,0.607056,-2.433399\C,0,4.199502,0.573675,-0.011185\C,0,4.60972,-0.505
623,-2.571978\C,0,5.028239,-0.546659,-0.200941\C,0,5.25487,-1.099848,-
1.475596\H,0,4.772085,-0.930369,-3.570268\H,0,5.51937,-0.993052,0.6715
53\C,0,4.055848,1.164869,1.393251\H,0,3.328292,1.991669,1.340114\C,0,3
.065719,1.171691,-3.677018\C,0,6.161231,-2.312799,-1.673934\H,0,6.2690
61,-2.455423,-2.765843\C,0,4.07867,1.850014,-4.6221\H,0,4.640077,2.648
903,-4.105173\H,0,4.811855,1.119946,-5.012767\H,0,3.558926,2.302292,-5
.486941\C,0,5.525942,-3.596285,-1.098558\H,0,4.523369,-3.772963,-1.526
82\H,0,6.155679,-4.476369,-1.32565\H,0,5.421593,-3.531382,-0.001242\C,
0,7.570774,-2.086741,-1.09199\H,0,7.539758,-1.975452,0.00745\H,0,8.227
363,-2.94598,-1.321433\H,0,8.036886,-1.177579,-1.512361\C,0,3.51342,0.
142287,2.409768\H,0,2.549914,-0.27478,2.073623\H,0,4.223696,-0.687707,
2.563431\H,0,3.353245,0.625467,3.391174\C,0,5.393858,1.770977,1.86831\
H,0,5.272652,2.254528,2.855302\H,0,6.173441,0.992804,1.965637\H,0,5.76
2029,2.532045,1.156874\C,0,-6.50665,-2.305078,-0.636279\H,0,-6.9035,-1
.954115,-1.60761\C,0,-2.984238,-0.785342,2.712935\H,0,-2.107918,-0.116
009,2.682495\C,0,-4.436411,2.308541,-1.145392\H,0,-3.695381,2.948175,-
0.636755\C,0,-5.828334,-3.669326,-0.87526\H,0,-5.434519,-4.094306,0.06
6066\H,0,-6.553185,-4.393641,-1.289821\H,0,-4.990138,-3.578151,-1.5872
87\C,0,-7.697827,-2.44047,0.335877\H,0,-8.212391,-1.472595,0.472921\H,
0,-8.435106,-3.17108,-0.045115\H,0,-7.358514,-2.787602,1.32948\C,0,-3.
94362,2.1037,-2.591849\H,0,-3.803796,3.079395,-3.092643\H,0,-2.979041,
1.568869,-2.604373\H,0,-4.674644,1.526305,-3.1872\C,0,-5.782029,3.0614
54,-1.110249\H,0,-6.110339,3.242233,-0.070849\H,0,-5.690491,4.040447,-
1.615638\H,0,-6.578002,2.491145,-1.623836\C,0,-3.7976,-0.470912,3.9874
41\H,0,-4.691095,-1.120193,4.050463\H,0,-3.185461,-0.644375,4.891849\H
,0,-4.142518,0.57687,4.005848\C,0,-2.445339,-2.227208,2.763529\H,0,-1.
746052,-2.337831,3.612527\H,0,-3.251979,-2.970118,2.905597\H,0,-1.8934
44,-2.460962,1.841216\C,0,2.238764,0.098588,-4.414052\H,0,1.711329,0.5
52193,-5.273914\H,0,2.877604,-0.713339,-4.808015\H,0,1.486946,-0.33466
,-3.732971\H,0,2.35579,1.945617,-3.339931\C,0,2.470902,-3.847655,2.227
989\C,0,1.403329,-4.677978,2.613104\H,0,1.445933,-5.227791,3.557514\C,
0,0.28701,-4.800375,1.784289\H,0,-0.541542,-5.437941,2.102578\C,0,0.21
5969,-4.080365,0.568442\C,0,1.303201,-3.253965,0.193346\H,0,1.29202,-2
.710877,-0.756492\C,0,2.423249,-3.139493,1.017105\H,0,3.254463,-2.4997
16,0.71359\C,0,-0.960511,-4.186169,-0.310699\C,0,-1.822009,-5.404904,-
0.304773\H,0,-1.992835,-5.717057,0.738432\H,0,-1.306077,-6.241756,-0.8
09262\H,0,-2.791678,-5.226541,-0.790873\N,0,-1.215073,-3.15617,-1.0925
93\H,0,-0.715147,-2.269969,-0.85883\C,0,-2.132373,-3.042968,-2.175157\
C,0,-2.296664,-4.088646,-3.10463\H,0,-1.718634,-5.011408,-3.009131\C,0
,-3.178174,-3.916596,-4.178429\H,0,-3.305067,-4.726065,-4.904628\C,0,-
3.875709,-2.708045,-4.335567\C,0,-3.687856,-1.665267,-3.414718\H,0,-4.
226671,-0.721642,-3.532226\C,0,-2.816667,-1.823016,-2.331426\H,0,-2.68
8982,-1.020842,-1.600182\H,0,-4.559968,-2.575996,-5.180118\C,0,3.65043
1,-3.691314,3.15736\F,0,3.965689,-4.854248,3.779991\F,0,4.76964,-3.267
415,2.51348\F,0,3.397941,-2.782498,4.137994\\Version=ES64L-G09RevD.01\
State=1-A\HF=-3513.6072361\RMSD=4.694e-09\Dipole=-2.3406352,-4.8416816
,-0.8551587\Quadrupole=-15.7819396,34.2362665,-18.4543269,17.4995955,3
.8230971,9.5584936\PG=C01 [X(C65H69F3N1O4P1)]\\@

Conf1

1\1\GINC-WORKER0\SP\RTPSSTPSS\def2SVP\C65H69F3N1O4P1\JHIOE\03-May-2019
\0\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(sm
d,solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,-0.1
557,0.028222,-0.404327\O,0,1.034305,1.017155,0.250479\O,0,-1.355159,1.

188475,-0.6433\O,0,-0.530209,-0.936561,0.700594\O,0,0.183359,-0.514408
,-1.774104\C,0,0.393253,3.299134,-0.110794\C,0,1.30526,2.254665,-0.292
474\C,0,2.568805,2.423345,-0.942064\C,0,2.862148,3.669558,-1.478649\H,
0,3.828386,3.833796,-1.967563\C,0,1.92649,4.744088,-1.429899\C,0,0.667
692,4.562914,-0.747408\C,0,-0.267846,5.641506,-0.757497\H,0,-1.240211,
5.50697,-0.274551\C,0,0.031208,6.843353,-1.382511\H,0,-0.707192,7.6528
43,-1.383637\C,0,1.282976,7.030157,-2.028179\H,0,1.508835,7.984999,-2.
515495\C,0,2.206662,5.996993,-2.054238\H,0,3.168592,6.122317,-2.564482
\C,0,-0.816325,3.069646,0.730805\C,0,-1.667015,2.001501,0.430859\C,0,-
2.878553,1.738948,1.145862\C,0,-3.205035,2.58562,2.195993\H,0,-4.14491
4,2.437037,2.737278\C,0,-2.341262,3.642386,2.606023\C,0,-1.116176,3.88
3703,1.883101\C,0,-0.236643,4.89901,2.368046\H,0,0.716745,5.067136,1.8
5933\C,0,-0.566645,5.662152,3.478582\H,0,0.128186,6.430922,3.834421\C,
0,-1.793328,5.450725,4.163149\H,0,-2.044876,6.064018,5.035362\C,0,-2.6
58104,4.455761,3.735689\H,0,-3.597431,4.266446,4.267956\C,0,-3.77964,0
.618116,0.716539\C,0,-3.829991,-0.600796,1.44969\C,0,-4.590889,0.78875
3,-0.436324\C,0,-4.691504,-1.620095,1.00492\C,0,-5.439879,-0.261133,-0
.835948\C,0,-5.502026,-1.476216,-0.135516\H,0,-4.73146,-2.558536,1.568
422\H,0,-6.067118,-0.132375,-1.726602\C,0,3.530456,1.275315,-0.986271\
C,0,3.82094,0.619374,-2.214565\C,0,4.137424,0.825152,0.218055\C,0,4.71
9686,-0.463795,-2.211742\C,0,5.030773,-0.260542,0.166161\C,0,5.332317,
-0.925954,-1.03385\H,0,4.938829,-0.966815,-3.160942\H,0,5.5029,-0.6064
41,1.092955\C,0,3.872417,1.496681,1.567231\H,0,3.122172,2.289868,1.412
292\C,0,3.181291,1.045914,-3.538316\C,0,6.298984,-2.107645,-1.0475\H,0
,6.571764,-2.312424,0.004658\C,0,4.225817,1.683377,-4.477867\H,0,4.721
461,2.548645,-4.002138\H,0,5.010918,0.954727,-4.75356\H,0,3.747185,2.0
33534,-5.411077\C,0,7.594003,-1.764509,-1.812886\H,0,8.086158,-0.87211
5,-1.386459\H,0,8.310429,-2.605449,-1.767966\H,0,7.382266,-1.557994,-2
.878364\C,0,5.642027,-3.383376,-1.613068\H,0,5.355925,-3.252793,-2.672
831\H,0,6.342203,-4.23703,-1.557532\H,0,4.732707,-3.649656,-1.046039\C
,0,3.288852,0.507069,2.59567\H,0,2.377607,0.025965,2.203474\H,0,4.0172
31,-0.279703,2.857517\H,0,3.022097,1.03747,3.528488\C,0,5.147404,2.179
866,2.105152\H,0,4.934165,2.711636,3.050783\H,0,5.944468,1.440346,2.30
6374\H,0,5.541779,2.915111,1.380675\C,0,-6.436724,-2.594424,-0.589682\
H,0,-6.841123,-2.296143,-1.575466\C,0,-2.998057,-0.813155,2.71614\H,0,
-2.146913,-0.113425,2.663951\C,0,-4.56978,2.086302,-1.246454\H,0,-3.86
8821,2.779161,-0.750966\C,0,-5.702783,-3.938072,-0.773872\H,0,-5.29978
9,-4.312974,0.184768\H,0,-6.395246,-4.705015,-1.166459\H,0,-4.863237,-
3.839689,-1.483405\C,0,-7.62816,-2.742196,0.380478\H,0,-8.179365,-1.79
0317,0.482856\H,0,-8.335141,-3.512357,0.020536\H,0,-7.282093,-3.04317,
1.386737\C,0,-4.046794,1.85775,-2.678853\H,0,-3.944664,2.821913,-3.210
151\H,0,-3.058072,1.369159,-2.659884\H,0,-4.740689,1.227071,-3.264501\
C,0,-5.951515,2.771079,-1.251809\H,0,-6.299317,2.972195,-0.222491\H,0,
-5.904079,3.734575,-1.791845\H,0,-6.712577,2.143342,-1.750869\C,0,-3.8
28041,-0.483544,3.976057\H,0,-4.698113,-1.161798,4.058287\H,0,-3.21500
3,-0.603915,4.88848\H,0,-4.209753,0.551407,3.956255\C,0,-2.407022,-2.2
32036,2.820345\H,0,-1.695765,-2.281563,3.665131\H,0,-3.185242,-2.99627
3,3.002584\H,0,-1.856094,-2.485125,1.90232\C,0,2.442816,-0.120577,-4.2
26076\H,0,1.961765,0.232425,-5.157341\H,0,3.134351,-0.938971,-4.499565
\H,0,1.659541,-0.519405,-3.559581\H,0,2.423944,1.815169,-3.311775\C,0,
2.753475,-3.666009,2.220085\C,0,1.744699,-4.539596,2.664009\H,0,1.8582
41,-5.078951,3.608723\C,0,0.597825,-4.723986,1.889795\H,0,-0.182497,-5
.398351,2.251006\C,0,0.438043,-4.027124,0.668923\C,0,1.46248,-3.14812,
0.240117\H,0,1.383166,-2.617009,-0.713381\C,0,2.611394,-2.968032,1.010
755\H,0,3.39295,-2.287016,0.666075\C,0,-0.754834,-4.224603,-0.171695\C
,0,-1.542126,-5.491141,-0.109934\H,0,-1.666873,-5.784595,0.945374\H,0,
-0.99132,-6.309932,-0.607363\H,0,-2.533085,-5.382143,-0.572986\N,0,-1.
085749,-3.235572,-0.977848\H,0,-0.633327,-2.31637,-0.779619\C,0,-2.017
458,-3.206336,-2.052753\C,0,-2.147414,-4.295525,-2.936959\H,0,-1.53488
8,-5.191181,-2.807001\C,0,-3.037157,-4.20052,-4.013379\H,0,-3.136433,-
5.043912,-4.704422\C,0,-3.77718,-3.024977,-4.219234\C,0,-3.624733,-1.9
38685,-3.343391\H,0,-4.196524,-1.020355,-3.498816\C,0,-2.746607,-2.019
609,-2.25726\H,0,-2.646388,-1.182374,-1.5617\H,0,-4.467136,-2.952931,-
5.066411\C,0,3.98436,-3.469324,3.072543\F,0,4.412351,-4.634661,3.62075
4\F,0,5.024639,-2.952268,2.371115\F,0,3.749097,-2.619159,4.109412\\Ver
sion=ES64L-G09RevD.01\State=1-A\HF=-3513.6070822\RMSD=4.627e-09\Dipole
=-2.0930171,-4.9468465,-0.726474\Quadrupole=-17.7116987,36.4686815,-18
.7569828,15.2310487,3.3327362,7.6537515\PG=C01 [X(C65H69F3N1O4P1)]\\@

Conf2

1\1\GINC-WORKER1\SP\RTPSSTPSS\def2SVP\C65H69F3N1O4P1\JHIOE\29-Apr-2019
\0\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(sm
d,solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,-0.2
36562,-0.045898,-0.397723\O,0,0.904678,1.033761,0.208701\O,0,-1.51622,
1.028515,-0.607933\O,0,-0.512511,-1.037434,0.712839\O,0,0.113418,-0.56
7018,-1.772489\C,0,0.136418,3.254735,-0.270969\C,0,1.091063,2.244199,-

0.429053\C,0,2.308262,2.431029,-1.156682\C,0,2.523652,3.661757,-1.7614
64\H,0,3.461859,3.842531,-2.296178\C,0,1.547311,4.698722,-1.720239\C,0
,0.322501,4.492116,-0.986711\C,0,-0.668644,5.519444,-1.025277\H,0,-1.6
20374,5.361064,-0.509633\C,0,-0.44667,6.702754,-1.714347\H,0,-1.225241
,7.473417,-1.73428\C,0,0.778094,6.921123,-2.400713\H,0,0.943776,7.8627
81,-2.93553\C,0,1.750601,5.933654,-2.407053\H,0,2.690793,6.080322,-2.9
51079\C,0,-1.028296,3.017959,0.627958\C,0,-1.826385,1.887144,0.428713\
C,0,-2.990881,1.604768,1.210678\C,0,-3.332338,2.504537,2.211264\H,0,-4
.238403,2.335486,2.801935\C,0,-2.521347,3.636231,2.514032\C,0,-1.33467
,3.891031,1.734328\C,0,-0.497637,4.982444,2.119314\H,0,0.43003,5.16458
8,1.569596\C,0,-0.83612,5.803813,3.18485\H,0,-0.17429,6.631298,3.46354
7\C,0,-2.028946,5.577497,3.92252\H,0,-2.288806,6.237367,4.757489\C,0,-
2.849202,4.509766,3.594575\H,0,-3.760861,4.309254,4.169092\C,0,-3.8176
73,0.385815,0.928676\C,0,-3.787291,-0.724325,1.815908\C,0,-4.646409,0.
352425,-0.225963\C,0,-4.610031,-1.832621,1.536261\C,0,-5.443093,-0.782
296,-0.464568\C,0,-5.451046,-1.882604,0.412208\H,0,-4.604621,-2.687472
,2.223077\H,0,-6.086772,-0.799138,-1.352063\C,0,3.329079,1.334835,-1.2
08798\C,0,3.541032,0.603182,-2.407464\C,0,4.100043,1.043532,-0.050114\
C,0,4.546428,-0.38295,-2.428083\C,0,5.080818,0.037022,-0.117228\C,0,5.
329799,-0.682172,-1.301014\H,0,4.726485,-0.941431,-3.354682\H,0,5.6732
51,-0.182341,0.778561\C,0,3.923831,1.833099,1.249098\H,0,3.09951,2.550
103,1.098758\C,0,2.722742,0.871217,-3.672823\C,0,6.40206,-1.767185,-1.
370679\H,0,6.516078,-2.03477,-2.438142\C,0,3.541416,1.685531,-4.696952
\H,0,3.888569,2.642932,-4.270858\H,0,4.433052,1.11978,-5.0263\H,0,2.93
2058,1.910679,-5.591685\C,0,5.962923,-3.041035,-0.617914\H,0,5.000351,
-3.421018,-1.003573\H,0,6.718457,-3.840324,-0.732414\H,0,5.841527,-2.8
42362,0.461284\C,0,7.770775,-1.271831,-0.863884\H,0,7.739579,-1.03336,
0.215032\H,0,8.541954,-2.050161,-1.009857\H,0,8.093612,-0.363328,-1.40
3232\C,0,3.531986,0.930157,2.434056\H,0,2.612557,0.364304,2.209968\H,0
,4.335683,0.214597,2.678504\H,0,3.346232,1.541903,3.336083\C,0,5.18821
9,2.659229,1.565898\H,0,5.033078,3.272306,2.472691\H,0,6.06062,2.00409
7,1.745816\H,0,5.439804,3.338303,0.731315\C,0,-6.356397,-3.088746,0.17
3003\H,0,-6.190716,-3.786456,1.015538\C,0,-2.915359,-0.732109,3.073815
\H,0,-2.159449,0.062063,2.951015\C,0,-4.725978,1.542102,-1.184907\H,0,
-4.017229,2.308352,-0.828277\C,0,-7.844955,-2.683964,0.187495\H,0,-8.0
78355,-1.993741,-0.644108\H,0,-8.492834,-3.572965,0.078081\H,0,-8.1119
97,-2.178329,1.132775\C,0,-5.99832,-3.836377,-1.1267\H,0,-4.941665,-4.
156472,-1.12568\H,0,-6.630526,-4.735968,-1.243219\H,0,-6.157644,-3.195
992,-2.013131\C,0,-4.303455,1.166589,-2.618207\H,0,-4.296355,2.064227,
-3.263617\H,0,-3.290104,0.73129,-2.62572\H,0,-5.003633,0.439409,-3.068
701\C,0,-6.130122,2.18092,-1.158562\H,0,-6.410424,2.48196,-0.133032\H,
0,-6.159773,3.081209,-1.799732\H,0,-6.899228,1.477674,-1.528137\C,0,-3
.759039,-0.404166,4.324756\H,0,-4.525478,-1.183423,4.495419\H,0,-3.118
647,-0.354096,5.224932\H,0,-4.280854,0.563038,4.223642\C,0,-2.150654,-
2.055985,3.267906\H,0,-1.462056,-1.969444,4.128811\H,0,-2.83244,-2.900
768,3.477715\H,0,-1.551697,-2.283068,2.37257\C,0,2.178236,-0.421069,-4
.311709\H,0,1.535029,-0.170271,-5.175581\H,0,2.990827,-1.071116,-4.685
221\H,0,1.56946,-0.979699,-3.582839\H,0,1.849256,1.476626,-3.375572\C,
0,2.973319,-3.287961,2.437882\C,0,2.143052,-4.388319,2.709381\H,0,2.25
7674,-4.9484,3.641225\C,0,1.168968,-4.766813,1.782596\H,0,0.519495,-5.
615164,2.013483\C,0,0.998704,-4.033906,0.585349\C,0,1.847161,-2.930653
,0.324634\H,0,1.76149,-2.369669,-0.611014\C,0,2.831161,-2.564854,1.242
324\H,0,3.485974,-1.719554,1.020515\C,0,-0.051156,-4.393746,-0.384685\
C,0,-0.489365,-5.809127,-0.563172\H,0,-0.510855,-6.319714,0.412136\H,0
,0.24692,-6.348007,-1.187716\H,0,-1.479398,-5.877378,-1.03752\N,0,-0.5
72144,-3.410173,-1.087105\H,0,-0.332561,-2.4392,-0.788518\C,0,-1.48571
,-3.45918,-2.180579\C,0,-1.320962,-4.37742,-3.23397\H,0,-0.482618,-5.0
78746,-3.231439\C,0,-2.219383,-4.350686,-4.308275\H,0,-2.091262,-5.059
248,-5.133066\C,0,-3.265199,-3.414662,-4.334149\C,0,-3.408247,-2.49220
8,-3.28491\H,0,-4.219143,-1.759295,-3.300753\C,0,-2.519127,-2.504153,-
2.205179\H,0,-2.632967,-1.797036,-1.379076\H,0,-3.964277,-3.397814,-5.
17681\C,0,3.996076,-2.849463,3.458565\F,0,4.386048,-3.863512,4.267653\
F,0,5.119646,-2.34756,2.876751\F,0,3.511337,-1.86847,4.267122\\Version
=ES64L-G09RevD.01\State=1-A\HF=-3513.6051754\RMSD=4.412e-09\Dipole=-0.
984357,-5.2731299,-1.1084255\Quadrupole=-20.6458054,40.6653368,-20.019
5315,5.6342927,1.3009998,11.1672736\PG=C01 [X(C65H69F3N1O4P1)]\\@

Conf3

1\1\GINC-WORKER0\SP\RTPSSTPSS\def2SVP\C65H69F3N1O4P1\JHIOE\29-Apr-2019
\0\\#p tpsstpss/def2svp int=ultrafine empiricaldispersion=gd3 scrf=(sm
d,solvent=ch2cl2,read,externaliteration,dovacuum)\\title\\0,1\P,0,-0.2
15755,-0.106495,-0.26437\O,0,0.805073,1.097644,0.317519\O,0,-1.591082,
0.823352,-0.555867\O,0,-0.420926,-1.072536,0.880618\O,0,0.223251,-0.62
9931,-1.617047\C,0,-0.155101,3.208807,-0.278492\C,0,0.897106,2.292495,
-0.367354\C,0,2.114161,2.569746,-1.064406\C,0,2.218561,3.783186,-1.731
222\H,0,3.14933,4.034092,-2.250631\C,0,1.137372,4.710568,-1.775643\C,0
,-0.076124,4.422921,-1.050294\C,0,-1.160512,5.346333,-1.152941\H,0,-2.

100214,5.124443,-0.638409\C,0,-1.042006,6.508075,-1.901674\H,0,-1.8897
88,7.198734,-1.970355\C,0,0.166643,6.806822,-2.586443\H,0,0.249618,7.7
30859,-3.169051\C,0,1.231401,5.921663,-2.525412\H,0,2.162998,6.132361,
-3.063047\C,0,-1.313749,2.897991,0.605278\C,0,-2.009285,1.697883,0.428
8\C,0,-3.18342,1.362973,1.173497\C,0,-3.625507,2.267193,2.129945\H,0,-
4.544937,2.056552,2.685873\C,0,-2.908569,3.463228,2.422736\C,0,-1.7212
88,3.781887,1.668398\C,0,-0.982585,4.948473,2.033062\H,0,-0.05555,5.18
0156,1.500733\C,0,-1.414579,5.777551,3.057891\H,0,-0.826738,6.663297,3
.323141\C,0,-2.608064,5.484422,3.770944\H,0,-2.942199,6.151213,4.57340
3\C,0,-3.334666,4.345664,3.460803\H,0,-4.245525,4.096217,4.017112\C,0,
-3.948558,0.107189,0.875488\C,0,-3.868803,-1.014306,1.743739\C,0,-4.79
4709,0.067099,-0.266001\C,0,-4.668601,-2.139908,1.465276\C,0,-5.566401
,-1.084703,-0.504806\C,0,-5.533473,-2.194154,0.359387\H,0,-4.62818,-3.
003453,2.139665\H,0,-6.226166,-1.106456,-1.380279\C,0,3.255502,1.59861
7,-1.013509\C,0,3.607774,0.833487,-2.159647\C,0,4.007545,1.471153,0.18
4839\C,0,4.723838,-0.020732,-2.088774\C,0,5.120859,0.609281,0.201149\C
,0,5.500935,-0.142635,-0.92284\H,0,4.996932,-0.604748,-2.975048\H,0,5.
707043,0.512397,1.122601\C,0,3.646134,2.239182,1.457609\H,0,2.77115,2.
872635,1.234487\C,0,2.820646,0.934106,-3.468423\C,0,6.716136,-1.06535,
-0.868853\H,0,7.123067,-1.001906,0.15736\C,0,3.594299,1.773033,-4.5079
22\H,0,3.825462,2.782141,-4.123993\H,0,4.551255,1.285705,-4.772915\H,0
,3.002681,1.886583,-5.435152\C,0,7.820077,-0.601155,-1.841175\H,0,8.11
6362,0.443588,-1.638479\H,0,8.718673,-1.237821,-1.743757\H,0,7.47711,-
0.659217,-2.890763\C,0,6.333497,-2.537114,-1.125652\H,0,5.924411,-2.67
3875,-2.143704\H,0,7.21987,-3.190703,-1.028809\H,0,5.573842,-2.88306,-
0.403866\C,0,3.239937,1.27877,2.594729\H,0,2.409898,0.625218,2.278455\
H,0,4.087441,0.643146,2.90619\H,0,2.907581,1.851799,3.480209\C,0,4.784
869,3.181753,1.898248\H,0,4.478726,3.769538,2.783171\H,0,5.695492,2.61
6988,2.170242\H,0,5.051505,3.889908,1.093096\C,0,-6.424048,-3.412612,0
.126616\H,0,-6.22807,-4.117733,0.956333\C,0,-2.967237,-1.009202,2.9799
05\H,0,-2.205772,-0.226729,2.820292\C,0,-4.917064,1.263502,-1.2122\H,0
,-4.232211,2.049067,-0.850705\C,0,-7.917837,-3.030287,0.181328\H,0,-8.
182025,-2.337361,-0.638761\H,0,-8.554877,-3.928129,0.08087\H,0,-8.1688
52,-2.535825,1.136871\C,0,-6.086637,-4.139273,-1.190255\H,0,-5.028467,
-4.452418,-1.213875\H,0,-6.715105,-5.041444,-1.306981\H,0,-6.267902,-3
.48772,-2.064439\C,0,-4.484565,0.913985,-2.649278\H,0,-4.51814,1.81428
2,-3.290017\H,0,-3.453276,0.522432,-2.663178\H,0,-5.152892,0.158212,-3
.10135\C,0,-6.340809,1.856595,-1.177086\H,0,-6.627319,2.138851,-0.1479
01\H,0,-6.400306,2.761612,-1.809437\H,0,-7.088471,1.13323,-1.551686\C,
0,-3.774533,-0.653682,4.247015\H,0,-4.548259,-1.419154,4.445163\H,0,-3
.111078,-0.60333,5.130273\H,0,-4.283267,0.320398,4.147841\C,0,-2.21290
7,-2.337861,3.177604\H,0,-1.484191,-2.236932,4.002867\H,0,-2.8961,-3.1
65669,3.4431\H,0,-1.65583,-2.604126,2.265903\C,0,2.444881,-0.444531,-4
.04607\H,0,1.834644,-0.314285,-4.95896\H,0,3.337705,-1.032221,-4.32887
1\H,0,1.84874,-1.016054,-3.31655\H,0,1.875113,1.457129,-3.245014\C,0,3
.57705,-3.109218,2.226137\C,0,2.905449,-4.30674,2.522041\H,0,3.210082,
-4.913086,3.379317\C,0,1.848517,-4.726475,1.71041\H,0,1.329748,-5.6555
89,1.958629\C,0,1.442489,-3.948641,0.600768\C,0,2.131864,-2.74359,0.31
8168\H,0,1.870065,-2.137691,-0.55503\C,0,3.188656,-2.327023,1.125832\H
,0,3.717206,-1.400798,0.88807\C,0,0.337532,-4.38652,-0.271363\C,0,-0.0
32042,-5.828658,-0.384952\H,0,-0.019952,-6.29377,0.613492\H,0,0.720615
,-6.360364,-0.995411\H,0,-1.02524,-5.965483,-0.835778\N,0,-0.298744,-3
.455419,-0.950094\H,0,-0.089745,-2.46108,-0.712138\C,0,-1.277017,-3.58
0132,-1.980723\C,0,-1.118987,-4.497792,-3.03607\H,0,-0.24214,-5.149321
,-3.077019\C,0,-2.076289,-4.533869,-4.058058\H,0,-1.953843,-5.242598,-
4.883579\C,0,-3.171584,-3.656342,-4.033541\C,0,-3.309396,-2.734209,-2.
983386\H,0,-4.159085,-2.04745,-2.958843\C,0,-2.365077,-2.687187,-1.952
582\H,0,-2.477094,-1.980858,-1.125075\H,0,-3.915123,-3.685407,-4.83691
9\C,0,4.714477,-2.641136,3.102026\F,0,5.297125,-3.658948,3.779686\F,0,
5.690759,-2.028637,2.380944\F,0,4.298728,-1.73857,4.032671\\Version=ES
64L-G09RevD.01\State=1-A\HF=-3513.6052377\RMSD=4.196e-09\Dipole=-0.677
3552,-5.204177,-1.1071978\Quadrupole=-20.2746366,41.2347341,-20.960097
5,0.1185029,1.4294712,8.9734658\PG=C01 [X(C65H69F3N1O4P1)]\\@

References

(1) Sorgenfrei, N.; Hioe, J.; Greindl, J.; Rothermel, K.; Morana, F.; Lokesh, N.; Gschwind, R. M. NMR Spectroscopic Characterization of Charge Assisted Strong Hydrogen Bonds in Brønsted Acid Catalysis. *J. Am. Chem. Soc.* **2016**, *138* (50), 16345–16354.

(2) Greindl, J.; Hioe, J.; Sorgenfrei, N.; Morana, F.; Gschwind, R. M. Brønsted Acid Catalysis-Structural Preferences and Mobility in Imine/Phosphoric Acid Complexes. *J. Am. Chem. Soc.* **2016**, *138* (49), 15965–15971.

(3) Aznar, F.; Valde, C. Modular Synthesis of Indoles from Imines and o -Dihaloarenes or o -Chlorosulfonates by a Pd-Catalyzed Cascade Process. *J. Am. Chem. Soc.* **2009**, *131* (8), 4031–4041.

(4) Schramm, Y.; Barrios-Landeros, F.; Pfaltz, A. Discovery of an Iridacycle Catalyst with Improved Reactivity and Enantioselectivity in the Hydrogenation of Dialkyl Ketimines. *Chem. Sci.* **2013**, *4*, 2760–2766.

(5) Harris, R. K.; Becker, E. D.; Cabral de Menezes, S. M.; Goodfellow, R.; Granger, P. NMR Nomenclature: Nuclear Spin Properties and Conventions for Chemical Shifts. IUPAC Recommendations 2001. International Union of Pure and Applied Chemistry. Physical Chemistry Division. Commission on Molecular Structure and Spectroscopy. *Magn. Reson. Chem.* **2002**, *40* (7), 489–505.

(6) Trigo-Mouriño, P.; Griesinger, C.; Lee, D. Label-Free NMR-Based Dissociation Kinetics Determination. *J. Biomol. NMR* **2017**, *69* (4), 229–235.

(7) Akke, M.; Palmer, A. G. Monitoring Macromolecular Motions on Microsecond to Millisecond Time Scales by R 1 ρ −R 1 Constant Relaxation Time NMR Spectroscopy. *J. Am. Chem. Soc.* **1996**, *118* (4), 911–912.

(8) Palmer, A. G.; Kroenke, C. D.; Loria, J. P. *Nuclear Magnetic Resonance Methods for Quantifying Microsecond-to-Millisecond Motions in Biological Macromolecules*; Elsevier Masson SAS, 2001; Vol. 339.

(9) Melikian, M.; Gramüller, J.; Hioe, J.; Greindl, J.; Gschwind, R. M. Brønsted Acid Catalysis – the Effect of 3,3′-Substituents on the Structural Space and the Stabilization of Imine/Phosphoric Acid Complexes. *Chem. Sci.* **2019**, *10*, 5226–5234.

(10) Jerschow, A.; Müller, N. Suppression of Convection Artifacts in Stimulated-Echo Diffusion Experiments. Double-Stimulated-Echo Experiments. *J. Magn. Reson.* **1997**, *125* (2), 372–375.

(11) Stejskal, E. O.; Tanner, J. E. Spin Diffusion Measurements: Spin Echoes in the Presence of a Time-Dependent Field Gradient. *J. Chem. Phys.* **1965**, *42* (1), 288–292.

(12) MacChioni, A.; Ciancaleoni, G.; Zuccaccia, C.; Zuccaccia, D. Determining Accurate Molecular Sizes in Solution through NMR Diffusion Spectroscopy. *Chem. Soc. Rev.* **2008**, *37* (3), 479–489.

(13) Chen, H. C.; Chen, S. H. Diffusion of Crown Ethers in Alcohols. *J. Phys. Chem.* **1984**, *88* (21), 5118–5121.

(14) Ben-Amotz, D.; Willis, K. G. Molecular Hard-Sphere Volume Increments. *J. Phys. Chem.* **1993**, *97* (29), 7736–7742.

(15) Zuccaccia, D.; Macchioni, A. An Accurate Methodology to Identify the Level of Aggregation in Solution by PGSE NMR Measurements: The Case of Half-Sandwich Diamino Ruthenium(II) Salts. *Organometallics* **2005**, *24* (14), 3476–3486.

(16) Reid, J. P.; Goodman, J. M. Goldilocks Catalysts: Computational Insights into the Role of the 3,3′ Substituents on the Selectivity of BINOL-Derived Phosphoric Acid Catalysts. *J. Am. Chem. Soc.* **2016**, *138* (25), 7910–7917.

(17) J. M. Tao; J. P. Perdew; V. N. Staroverov; G. E. Scuseria. Climbing the density functional ladder: Nonempirical meta-generalized gradient approximation designed for molecules and solids. *Phys. Rev. Lett.* **2003**, *91,* 146401.

(18) S. Grimme; J. Antony, S. Ehrlich; H. Krieg. A consistent and accurate ab initio parameterization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys*. **2010**, *132*, 154104.

(19) A. V. Marenich; C. J. Cramer; D. G. Truhlar. Universal solvation model based on solute electron density and a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions. *J. Phys. Chem. B*, **2009**, *113*, 6378-6396.

(20) S. Grimme. Improved second-order Møller–Plesset perturbation theory by separate scaling of parallel- and antiparallel-spin pair correlation energies. *J. Chem. Phys.*, **2003**, *118*, 9095.

(21) Gaussian 09, Revision D.01, M. J. Frisch; G. W. Trucks; H. B. Schlegel; G. E. Scuseria; M. A. Robb; J. R. Cheeseman; G. Scalmani; V. Barone; B. Mennucci; G. A. Petersson; H. Nakatsuji; M. Caricato; X. Li; H. P. Hratchian; A. F. Izmaylov; J. Bloino; G. Zheng; J. L. Sonnenberg; M. Hada; M. Ehara; K. Toyota; R. Fukuda; J. Hasegawa; M. Ishida; T. Nakajima; Y. Honda; O. Kitao; H. Nakai; T. Vreven; J. A. Montgomery, Jr.; J. E. Peralta; F. Ogliaro; M. Bearpark; J. J. Heyd; E. Brothers; K. N. Kudin; V. N. Staroverov; R. Kobayashi; J. Normand; K. Raghavachari; A. Rendell; J. C. Burant; S. S. Iyengar; J. Tomasi; M. Cossi; N. Rega; J. M. Millam; M. Klene; J. E. Knox; J. B. Cross; V. Bakken; C. Adamo; J. Jaramillo; R. Gomperts; R. E. Stratmann; O. Yazyev; A. J. Austin; R. Cammi; C. Pomelli; J. W. Ochterski; R. L. Martin; K. Morokuma; V. G. Zakrzewski; G. A. Voth; P. Salvador; J. J. Dannenberg; S. Dapprich; A. D. Daniels; Ö. Farkas; J. B. Foresman; J. V. Ortiz; J. Cioslowski; D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

(22) F. Neese. Software update: the ORCA program system, version 4.0. *WIREs Comput Mol Sci*, **2018**, 8:e1327. doi: 10.1002/wcms.1327

(23) S. Grimme; C. Bannwarth; P. Shushkov. A Robust and Accurate Tight-Binding Quantum Chemical Method forStructures, Vibrational Frequencies, and Noncovalent Interactions ofLarge Molecular Systems Parametrized for All spd-Block Elements(Z=1−86). *J. Chem. Theory Comput*. **2017**, *13,* 1989.