

Brønsted Acid Catalysis – The Effect of 3,3'-Substituents on the Structural Space and the Stabilization of Imine/Phosphoric Acid Complexes

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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- d_8 was refluxed over Na/Benzophenone under argon atmosphere. Freon mixtures were prepared from CDCl_3 and $\text{SbCl}_5/\text{SbF}_3$ according to literature procedures and stored in small lecture bottles.^[1,2] The catalysts were purchased from Sigma Aldrich or synthesized from the bisphenols according to the procedure of Klusmann et al.^[3]

Synthesis of Imine Substrates

The imines were prepared as described in literature.^[4–7] The toluene was used either in p.A. quality or was dried by refluxing over sodium. The ^{15}N -enriched aniline for the presented syntheses below, was purchased from Euriso-top GmbH and Sigma Aldrich.

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) 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. A concentration of 25 mmol, 50 mmol/L or 100 mM was used for all samples, depending on solubility at low temperatures.

Spectrometer data

NMR experiments were performed on Bruker Avance III HD 400 MHz spectrometer, equipped with 5 mm BBO BB-1H/D probe head with Z-Gradients and a Bruker Avance III HD 600 MHz spectrometer, equipped with a 5 mm TBI 1H/31P and a 5 mm CPPBBO BB-1H/19F. Triple resonance experiments were performed on the TBI probe head.. 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. For samples in freonic mixtures as solvents, 5 mm heavy wall (1.4 mm wall thickness) NMR tubes equipped with J. Young valves from Wilmad were used. NMR Data were processed, evaluated and plotted with TopSpin 3.2 software. Further plotting of the spectra was performed with Corel Draw X14 – X17 software. ^1H , ^{13}C chemical shifts were referenced to TMS or the respective solvent signals. The heteronuclei ^{15}N , ^{19}F and were referenced, employing $\nu(\text{X}) = \nu(\text{TMS}) \times \Xi_{\text{reference}} / 100 \%$ according to Harris et al.^[8] The following frequency ratios and reference compounds were used: $\Xi(^{15}\text{N}) = 10.132912$ (lq. NH_3) and $\Xi(^{19}\text{F}) = 94.094011$ (CCl_3F)

Pulse programs

All pulse programs used are standard Bruker NMR pulse programs.

Acquisition Parameters

^1H 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- ^1H , ^1H NOESY: Pulse program: noesygpqh/noesygpqhpp; Relaxation delay = 5 - 8 s, NS = 8-32, mixing time (D8) = 300.00 ms; TD = 4096; increments = 512 - 1k;

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

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

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

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

Dilution experiments for dimer identification

S1. Diluted spectra of TRIM/7

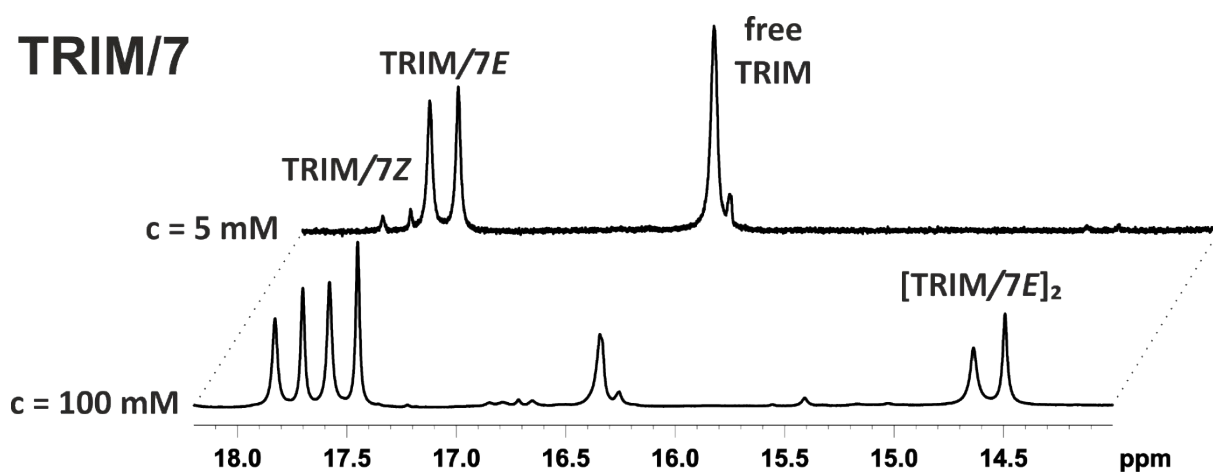


Figure S34: ¹H-spectra of TRIM/7 at 180 K in CD₂Cl₂ at 600 MHz with a concentration of 5 mM or 100 mM. The signal of [TRIM/7E]₂ disappears at lower concentration, corroborating the assignment as a dimeric species. The changing *E/Z* ratio of TRIM/7E and TRIM/7Z at 5 mM and 100 mM is caused by insufficient equilibration at room temperature before measuring.

1-naph/6

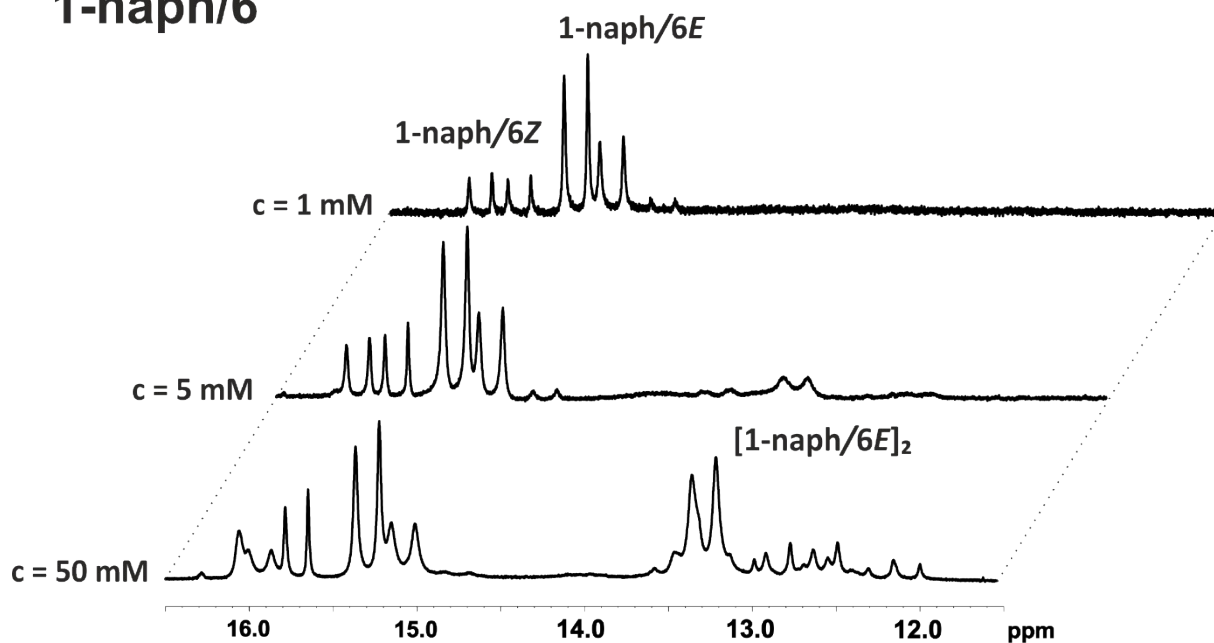


Figure S35: ¹H-spectra of 1-naph/6 at 180 K in CD₂Cl₂ at 600 MHz with a concentration of 1 mM, 5 mM or 50 mM. The signal of [1-naph/6E]₂ disappears at lower concentration, corroborating the assignment as a dimeric species.

9-phen/6

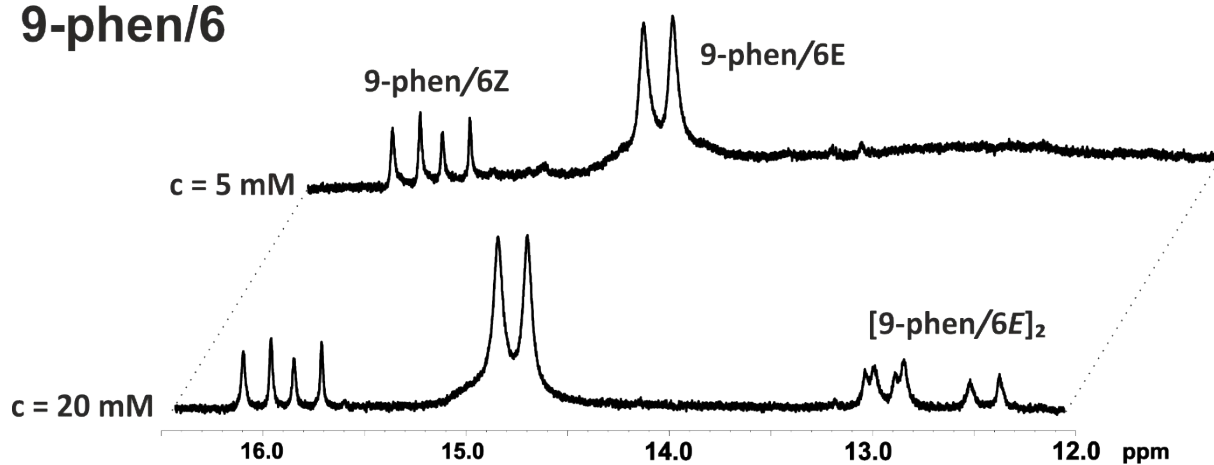


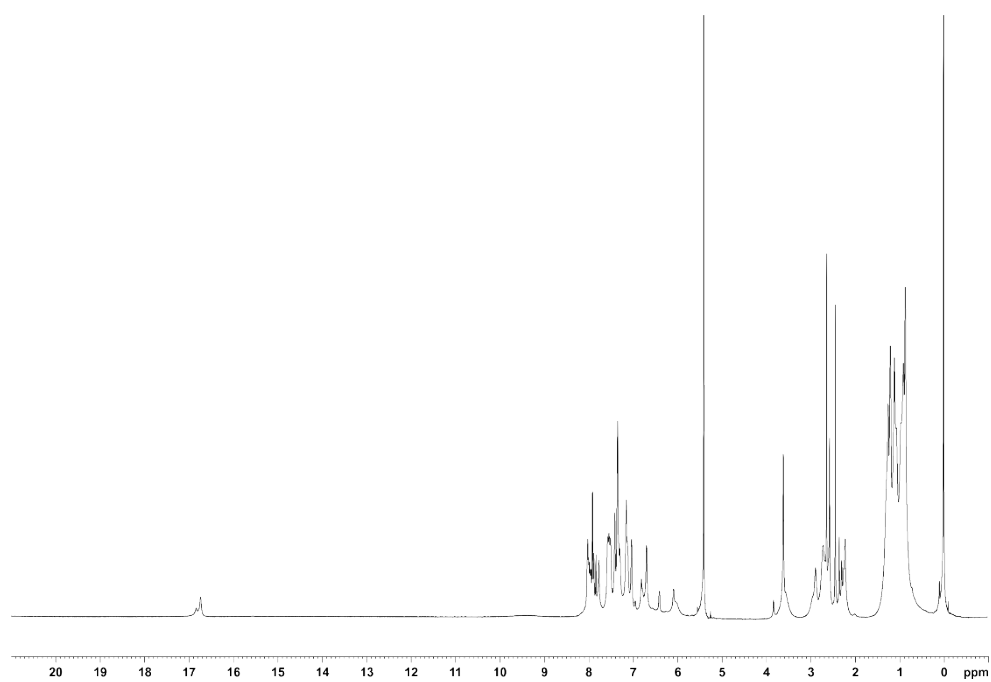
Figure S36: ^1H -spectra of 9-phen/6 at 180 K in CD_2Cl_2 at 600 MHz with a concentration of 5 mM or 20 mM. The signal of $[\text{9-phen/6E}]_2$ disappears at lower concentration, corroborating the assignment as a dimeric species.

S4 *E/Z* Ratios of CPA/imine complexes

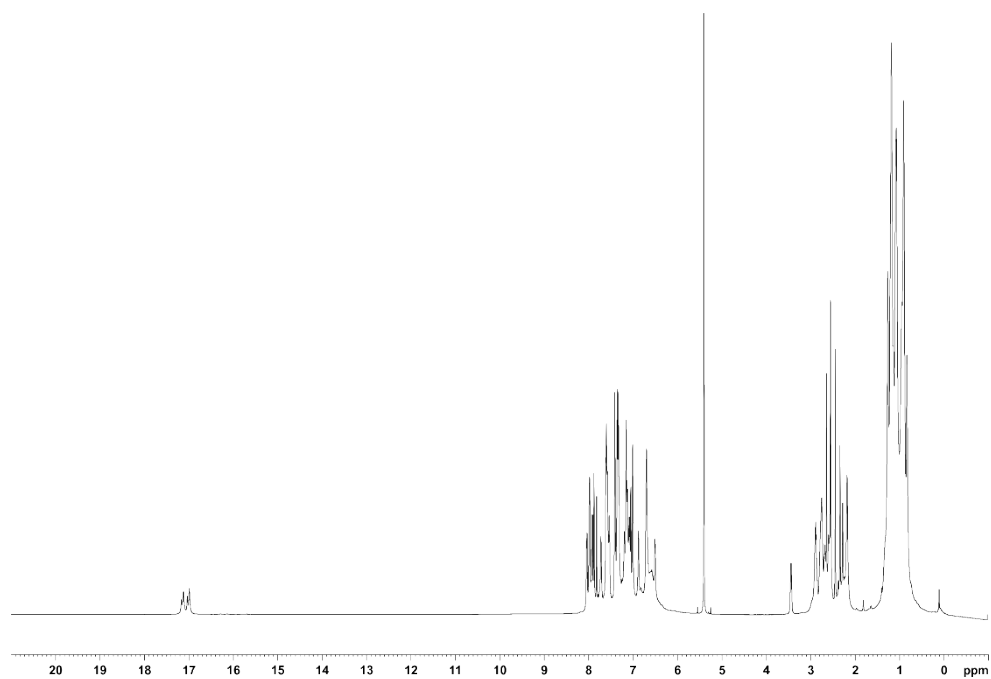
For the determination of the *E/Z* ratios of the different complexes, the integrals of the hydrogen bond protons were used. For overlapping signals, deconvolution was used. If the signals could not be separated, the integrals of the alpha-methyl groups of the imines were used instead.

	1	2	3	4	5	6	7
TRIP	n.d.	62:38	n.d.	n.d.	67:33	77:23	86:14
TiPSY	45:55	53:47	51:49	68:32	56:44	70:30	71:29
TRIFP	n.d.	n.d.	n.d.	83:17	70:30	81:19	69:30
TRIM	n.d.	n.d.	n.d.	n.d.	47:53	49:51	55:45

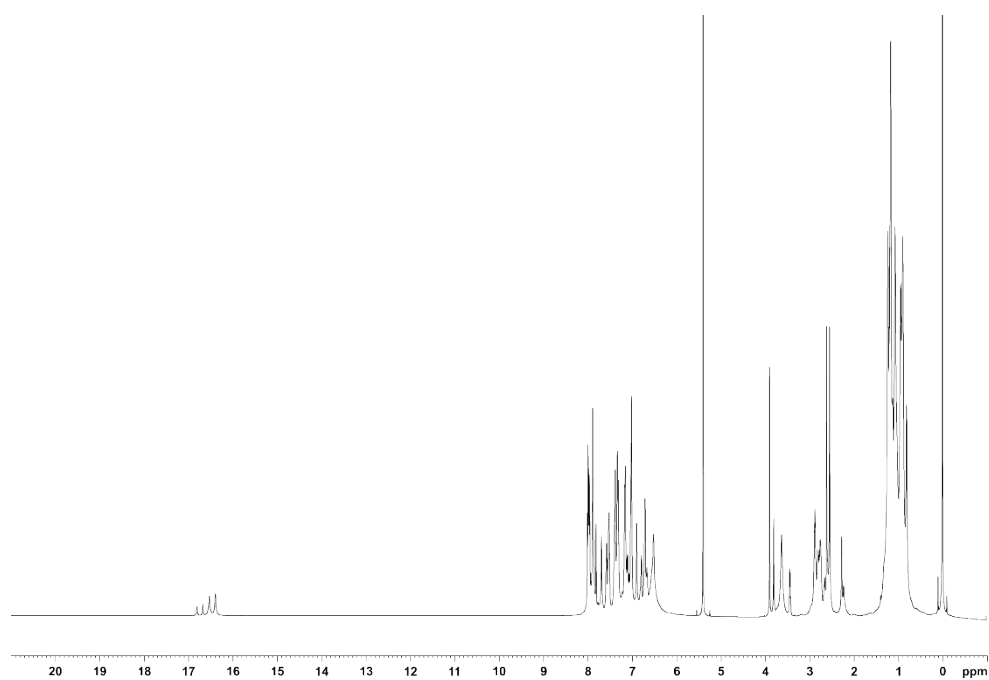
TRIP/2



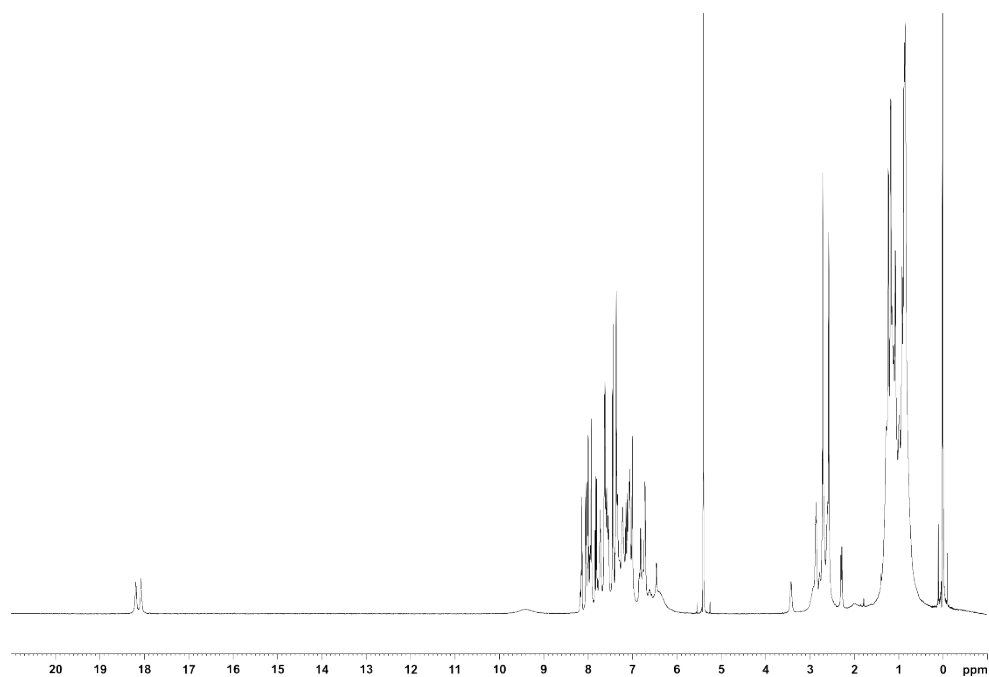
TRIP/5



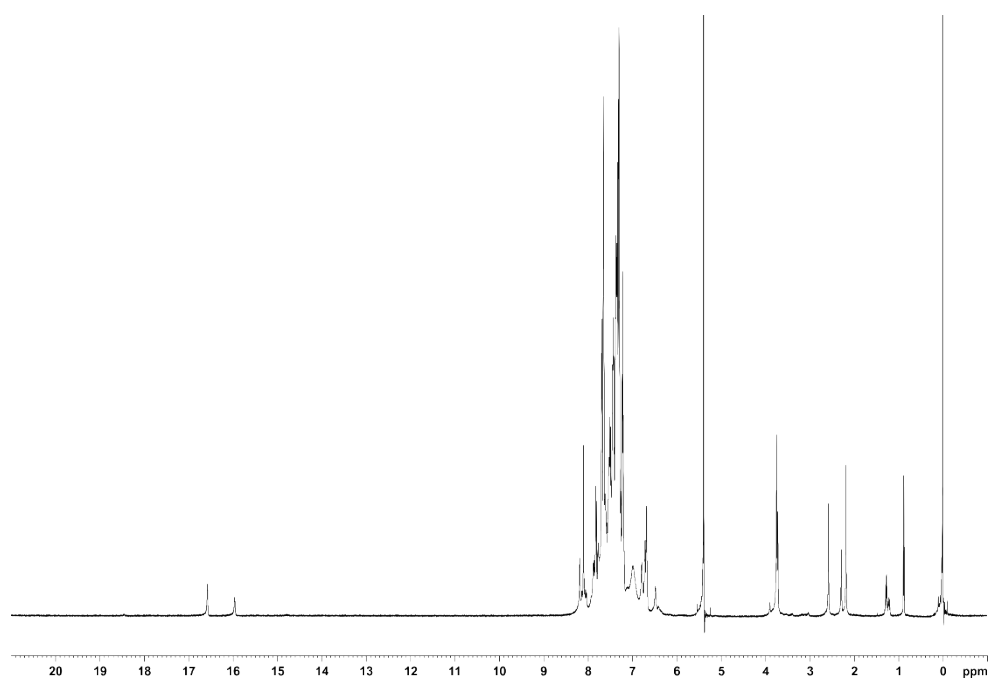
TRIP/6



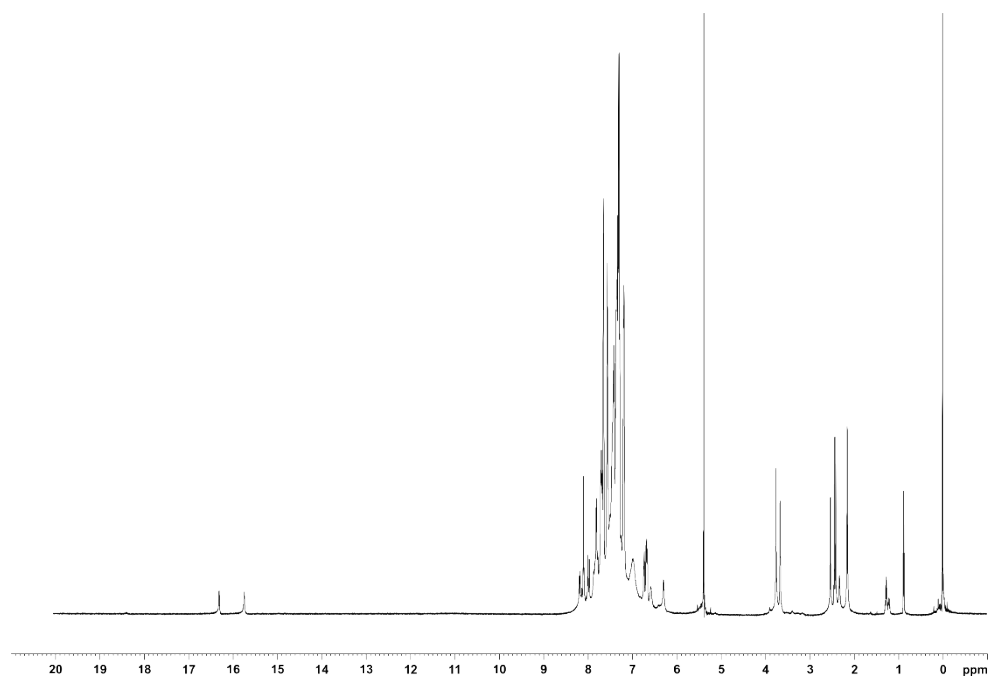
TRIP/7



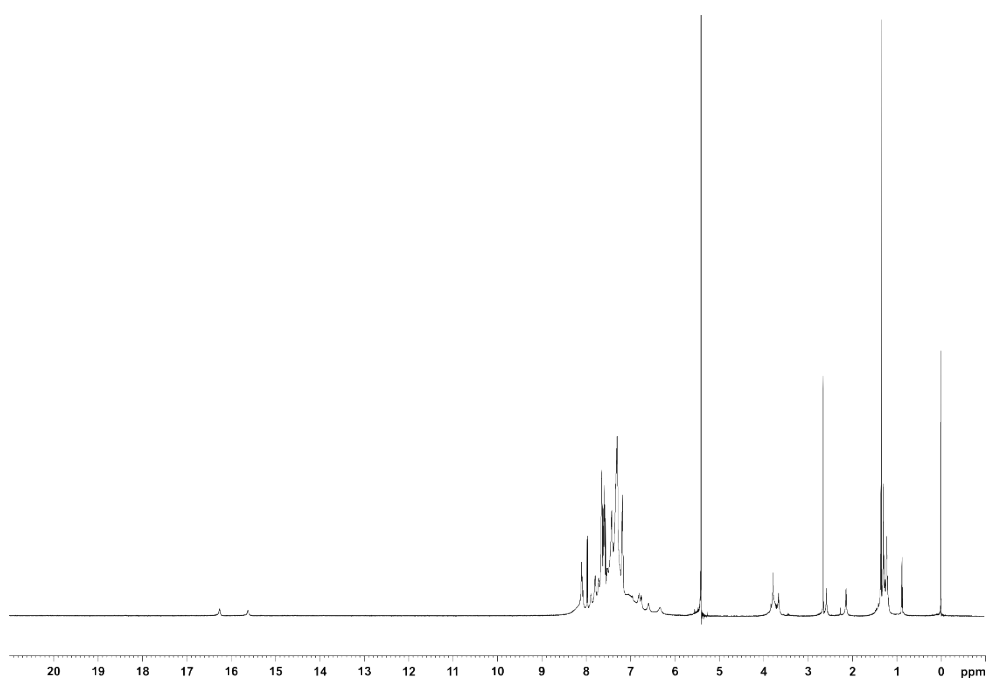
TiPSY/1



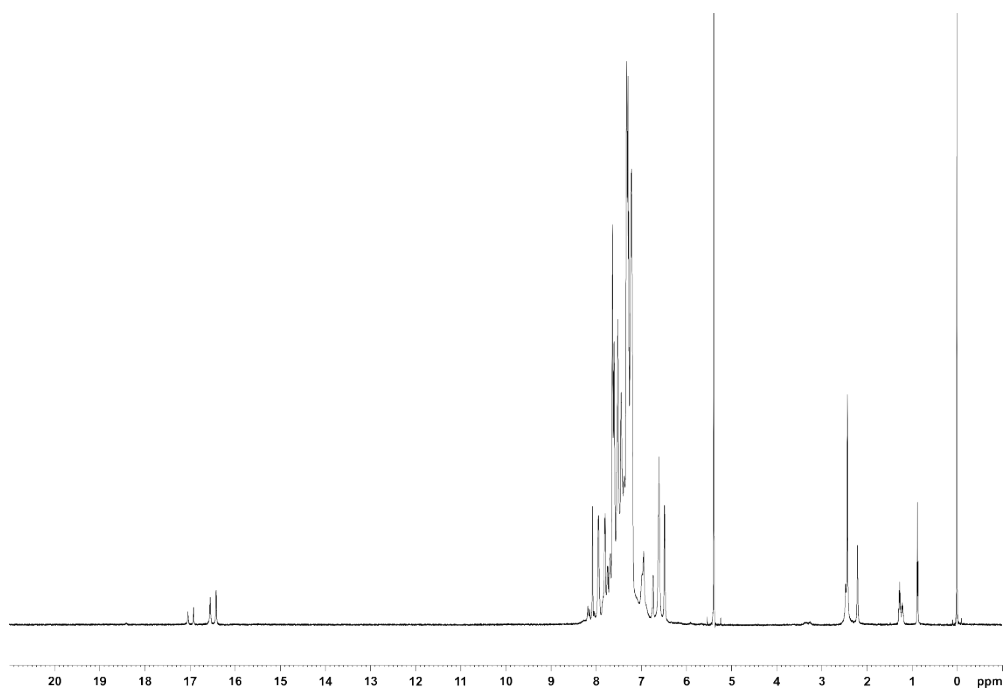
TiPSY/2



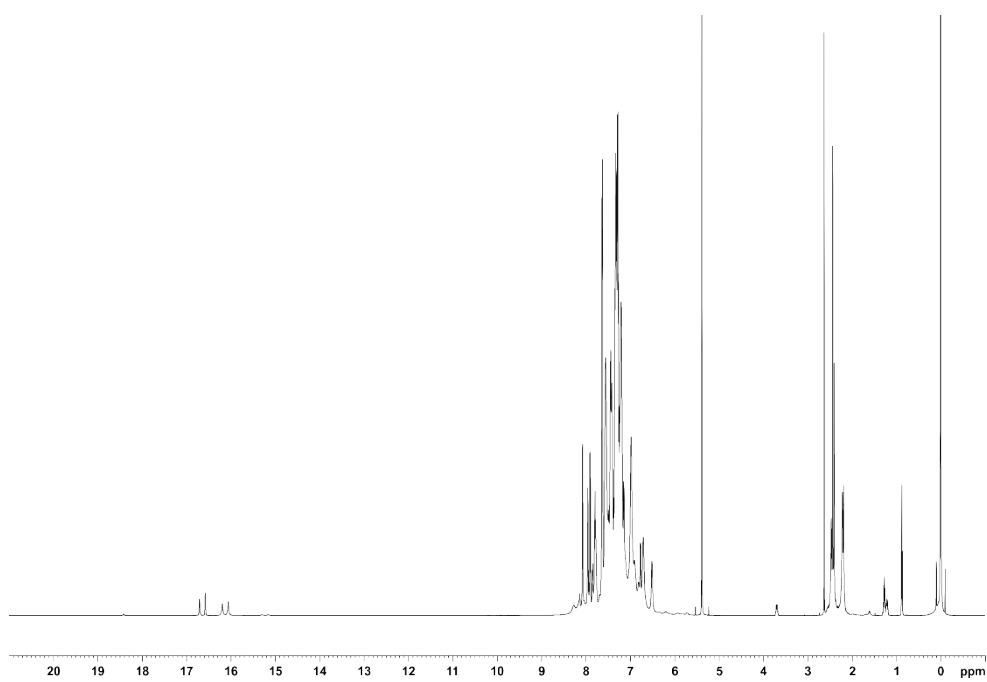
TiPSY/3



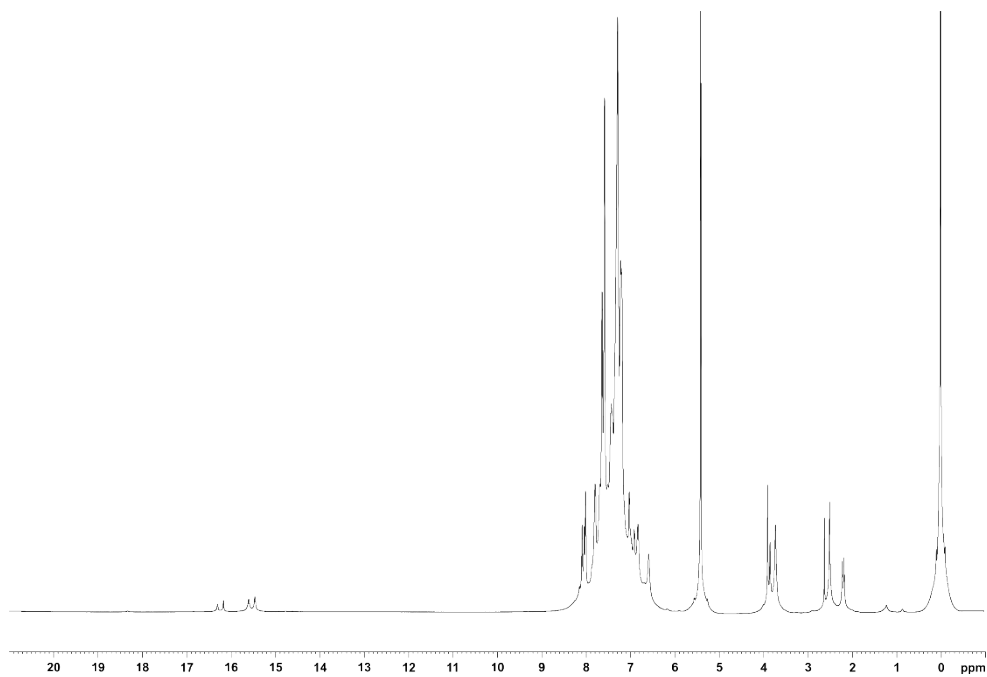
TiPSY/4



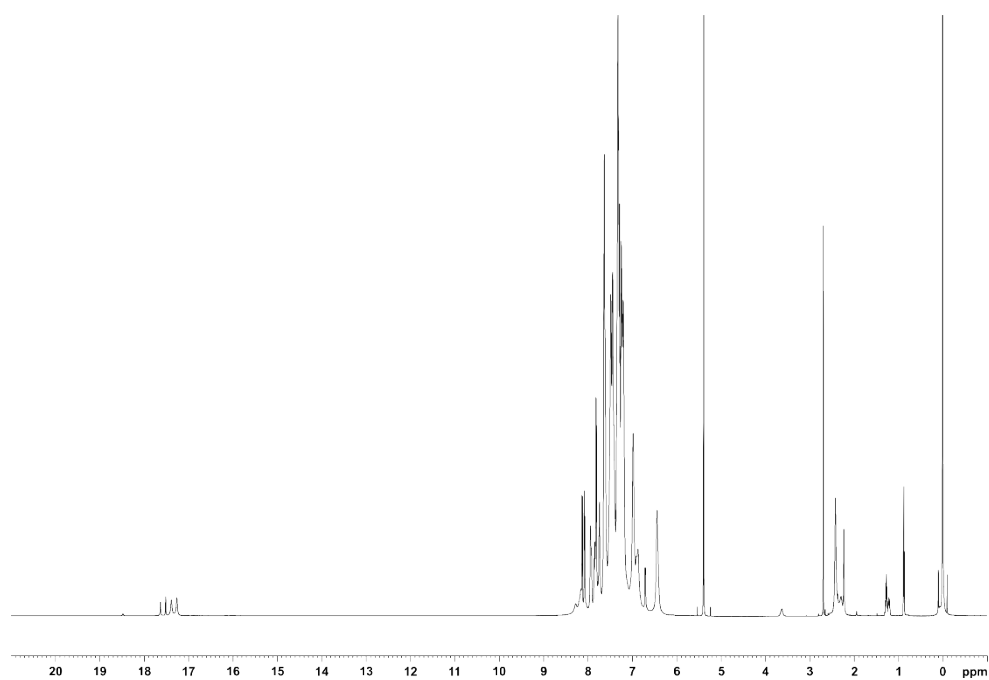
TiPSY/5



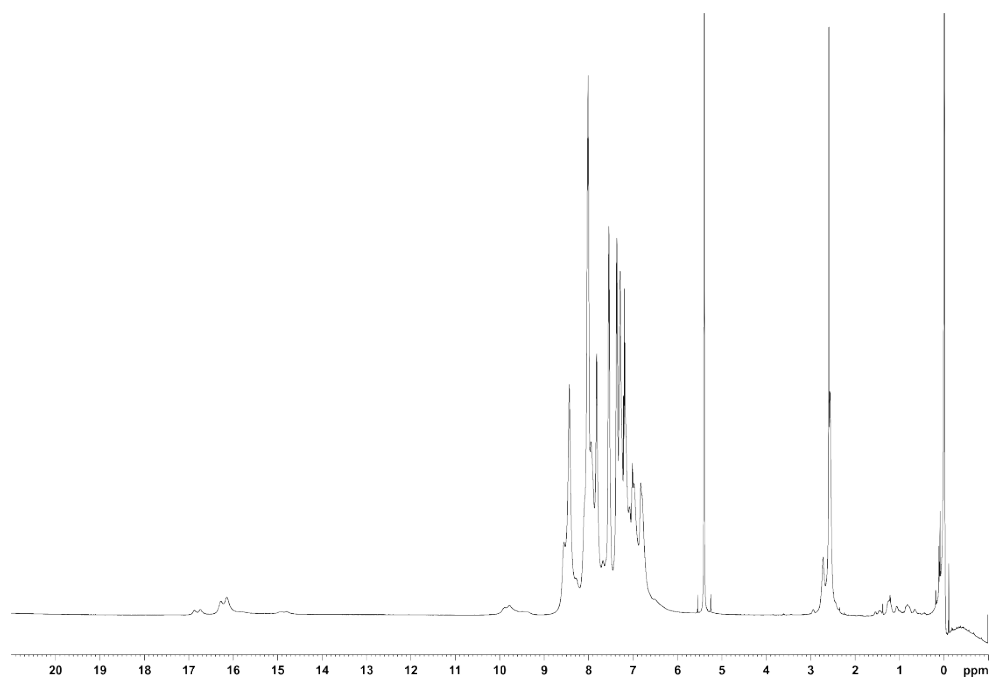
TiPSY/6



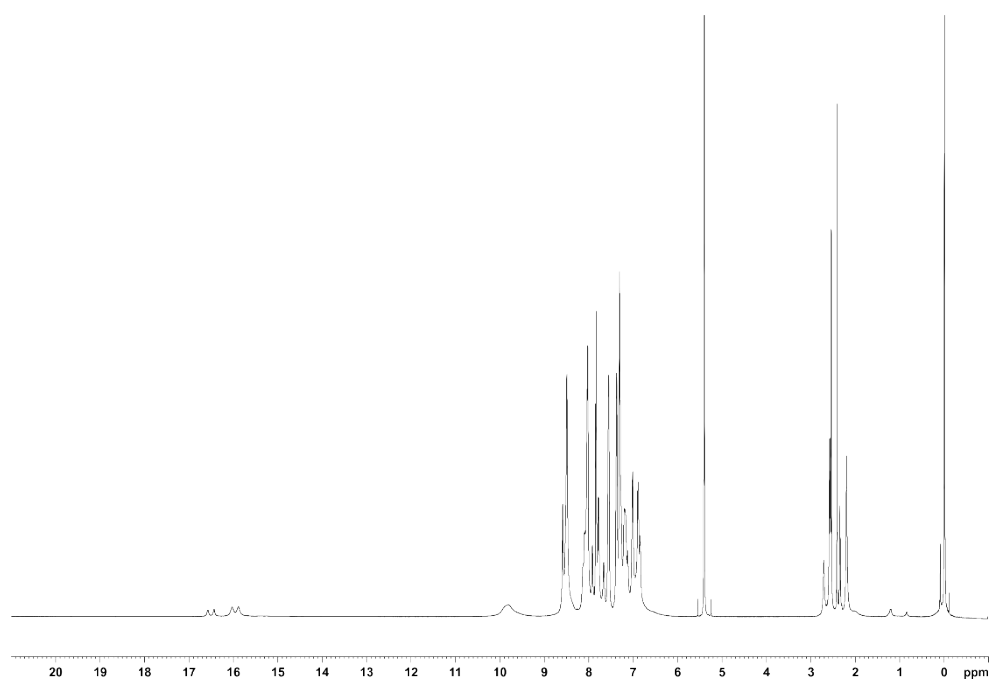
TiPSY/7



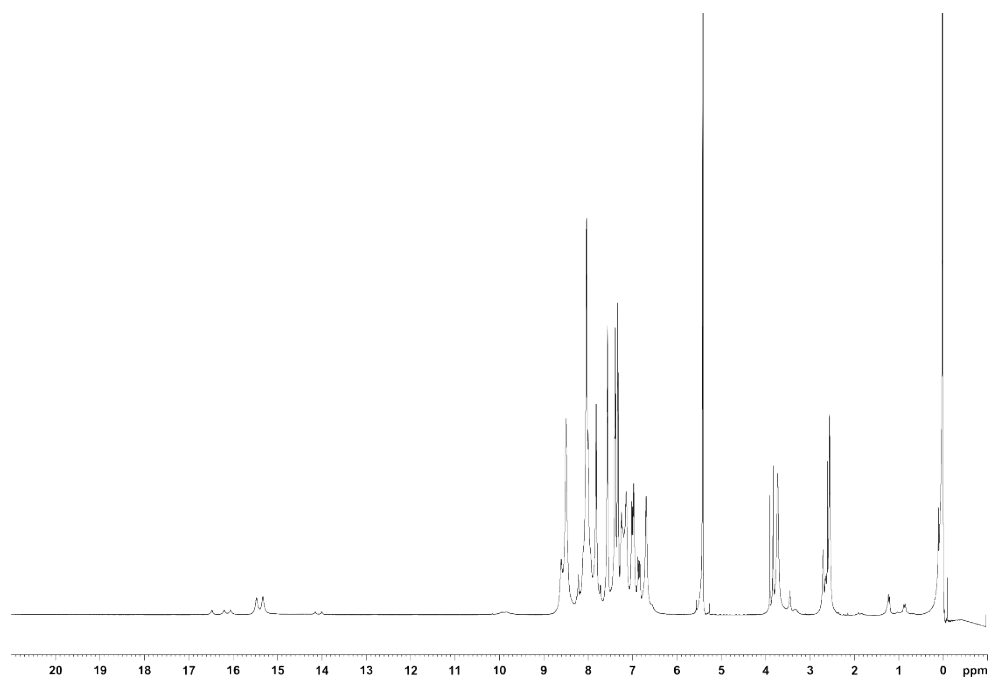
TRIFP/4



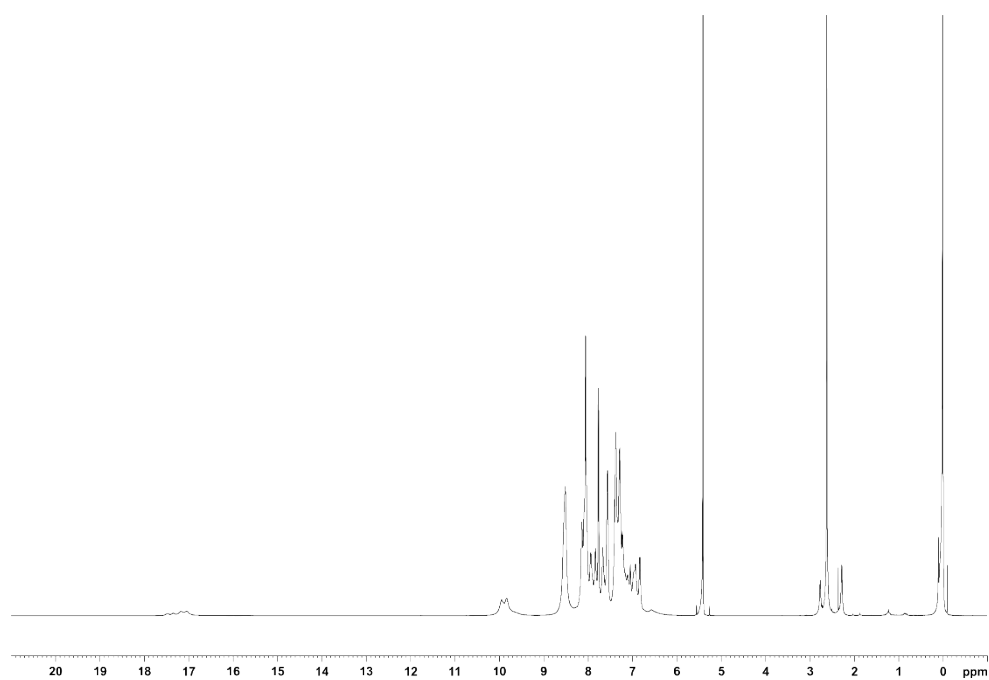
TRIFP/5



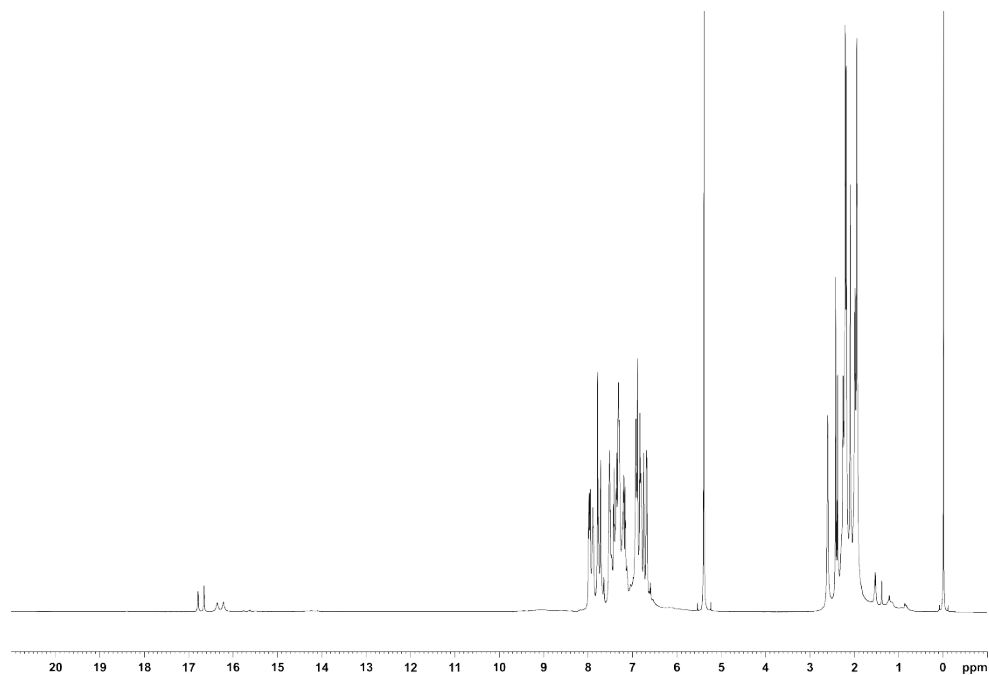
TRIFP/6



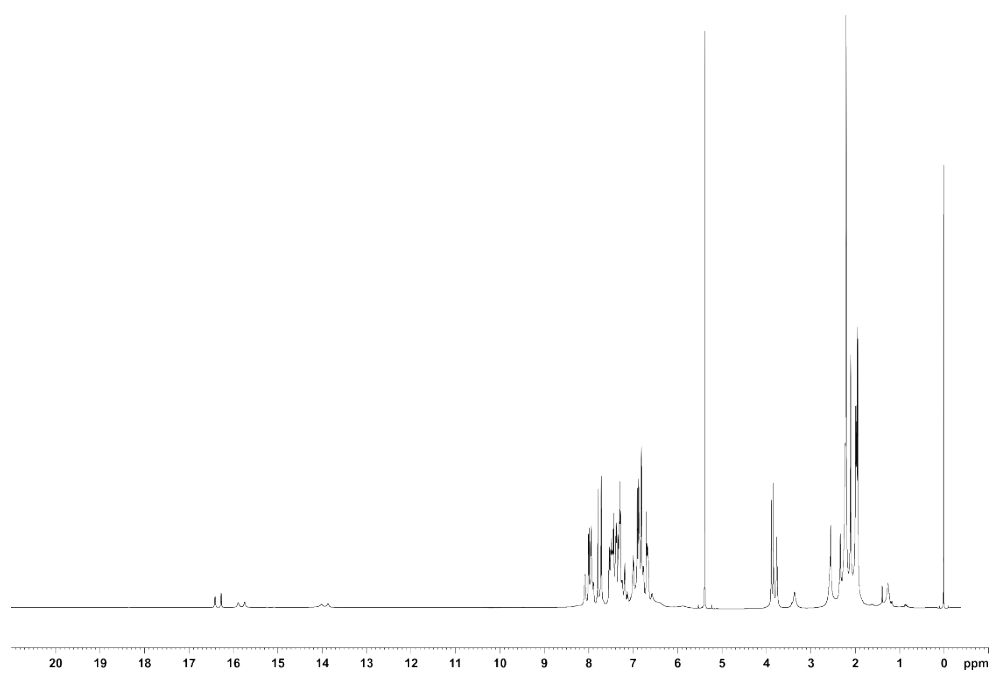
TRIFP/7



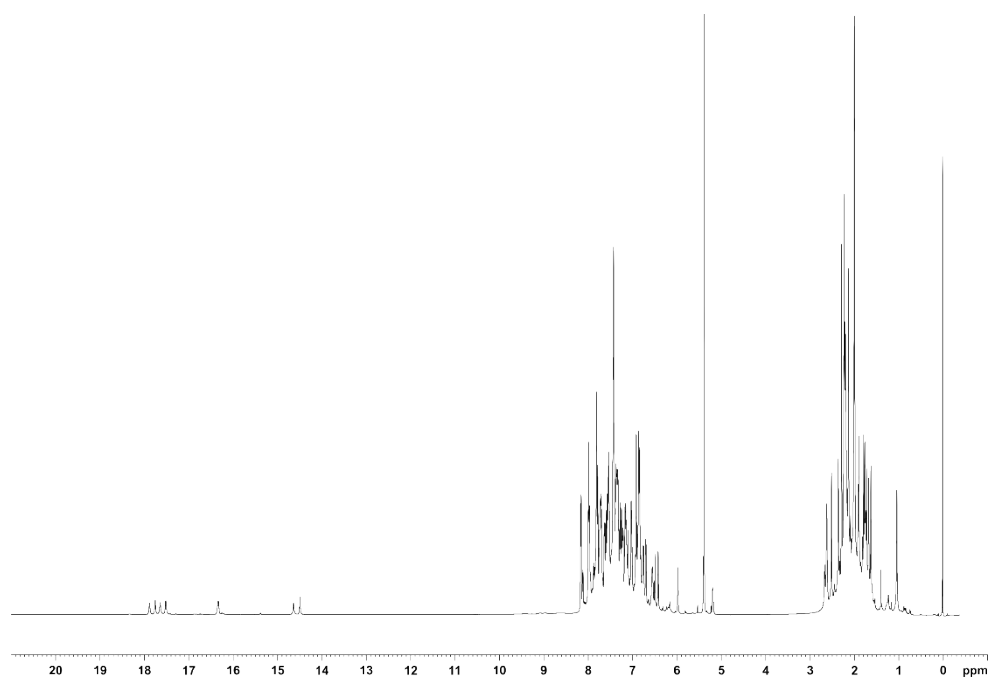
TRIM/5



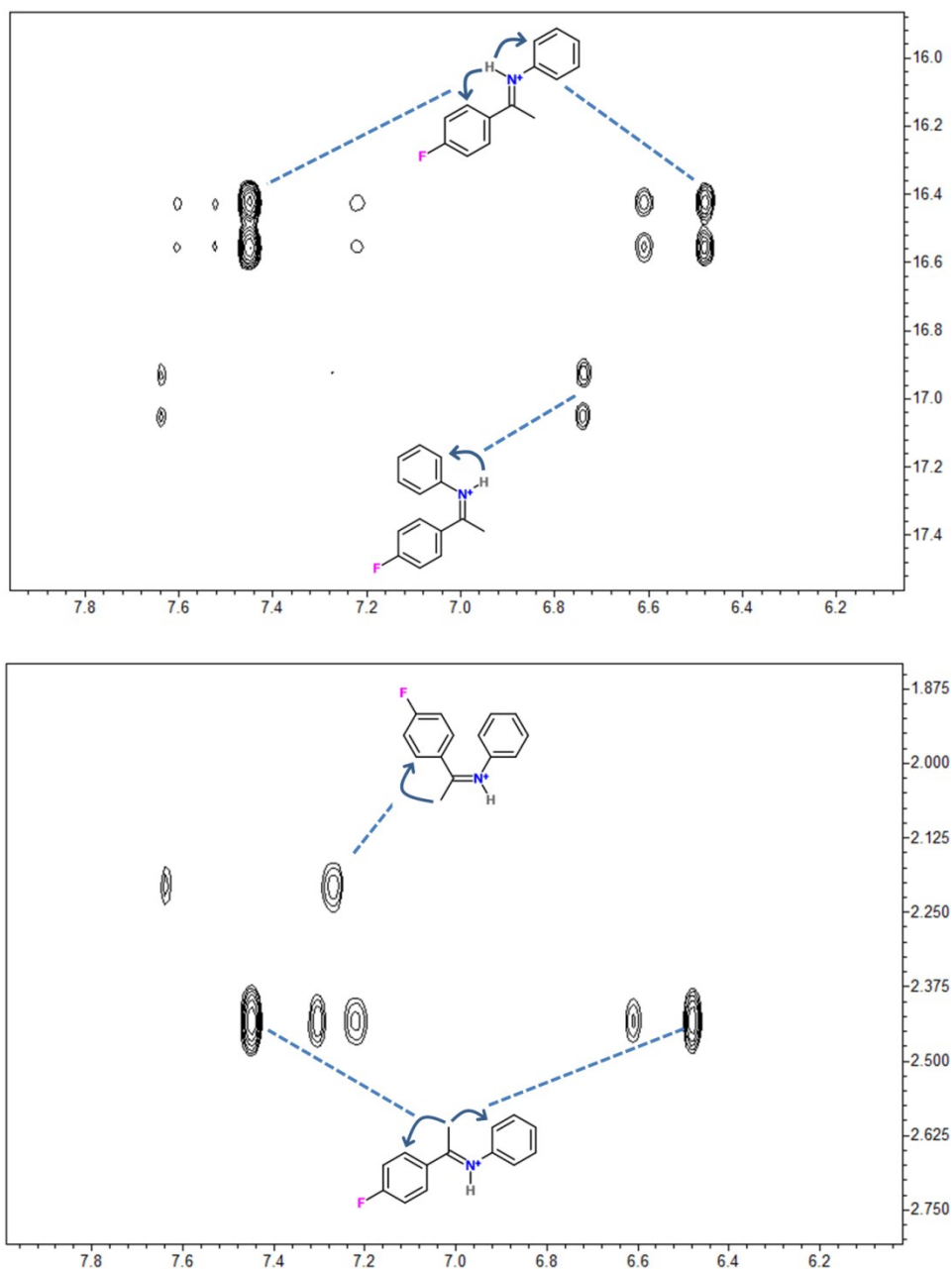
TRIM/6



TRIM/7



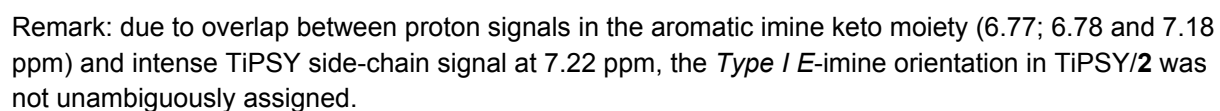
S5 Identification of *E*- and *Z*-imines inside the complex



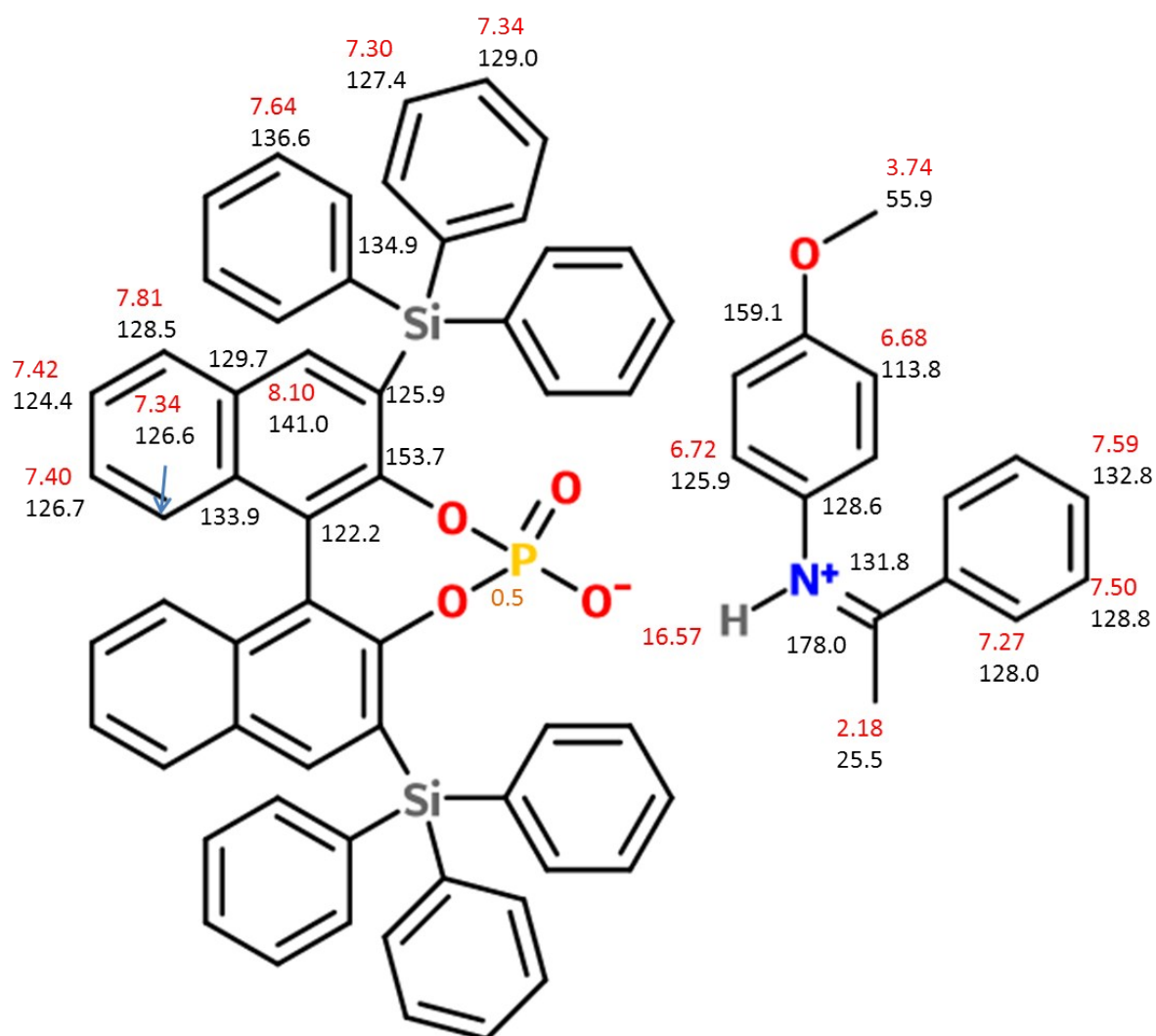
Selected areas from a NOESY experiment allowing identification of *E*- and *Z*-isomers in complex with TiPSY. The aromatic/H-bond section is shown in the upper panel and the aromatic/methyl section is shown in the lower panel. Similar patterns can be observed for the other TiPSY/imine complexes. The two intense *E*-imine cross-peaks from respectively the H-bond proton and α -methyl proton toward the same two aromatic protons. On the other hand only one intense cross peak can be observed for the *Z*-imine towards two different aromatic protons.

NMR Parameters: mixing time 300 ms, Time domain: 2k x 256, recycling delay: 2s, Number of scans: 8. Experiment time: 2h50min.

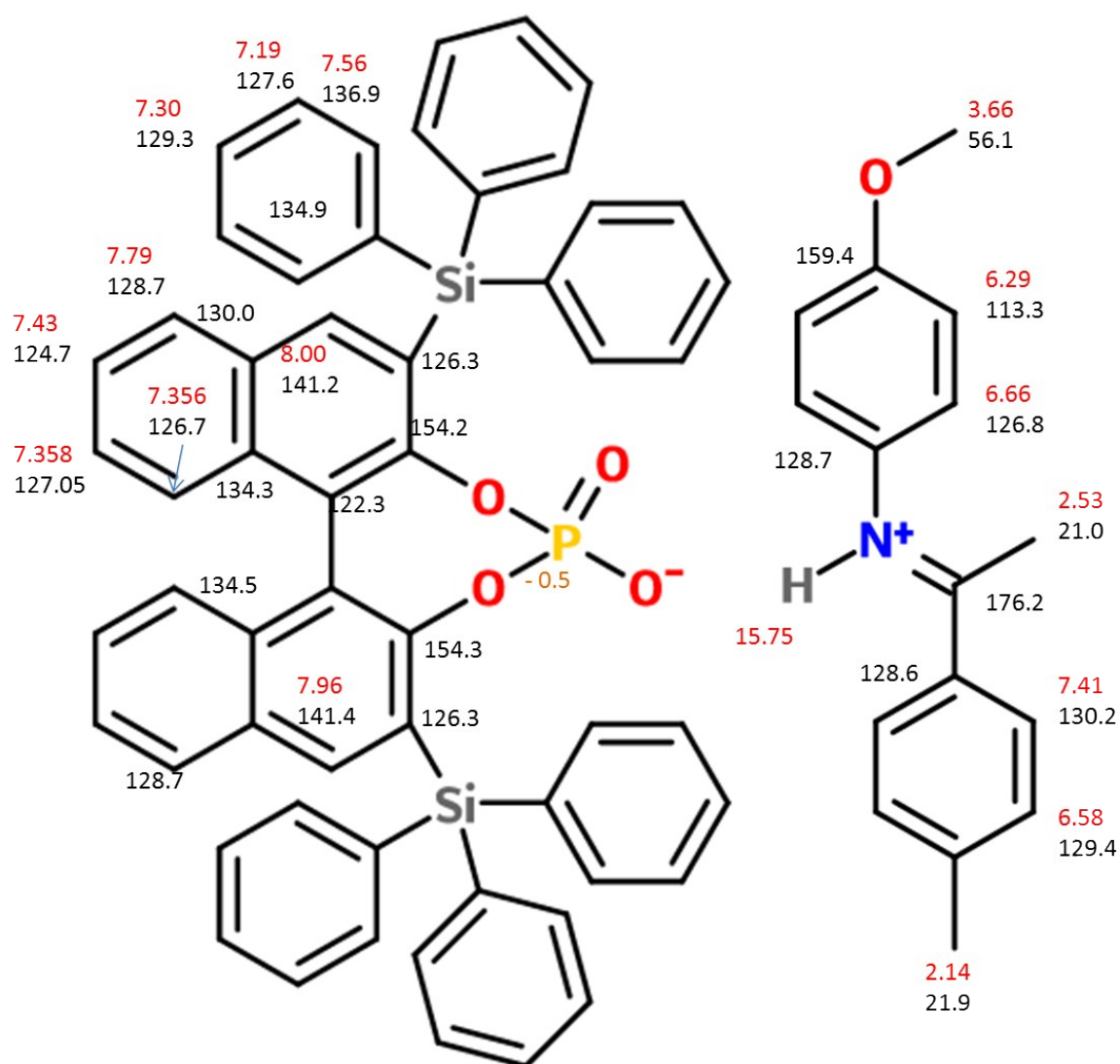
S6. Complex (TiPSY/1E)



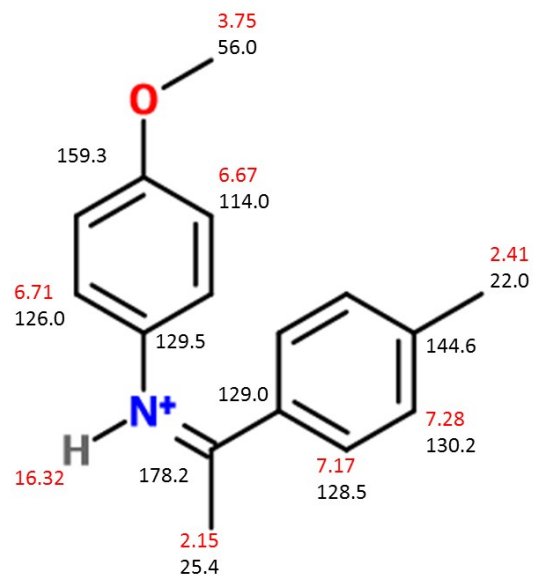
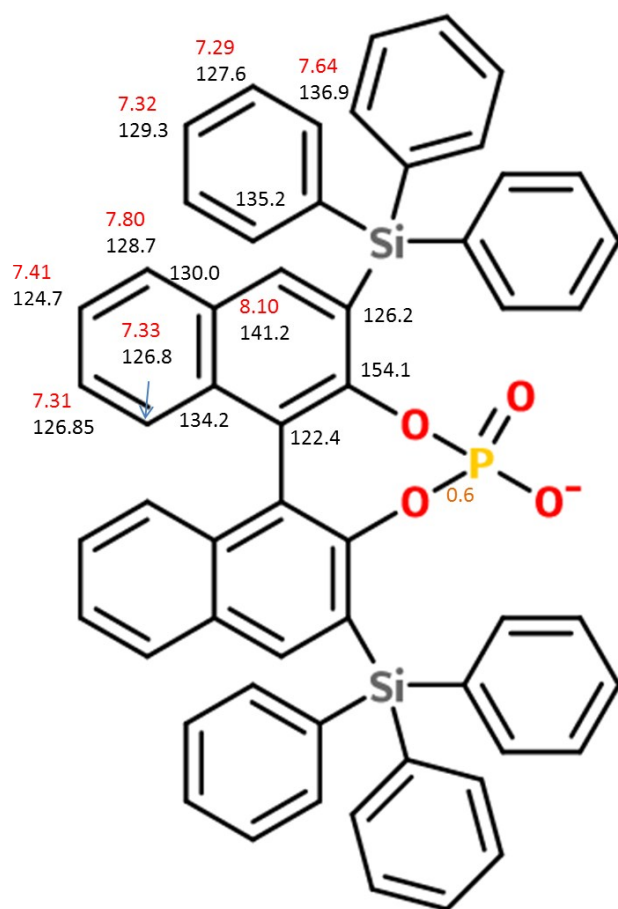
S7. Complex (TiPSY/1Z)



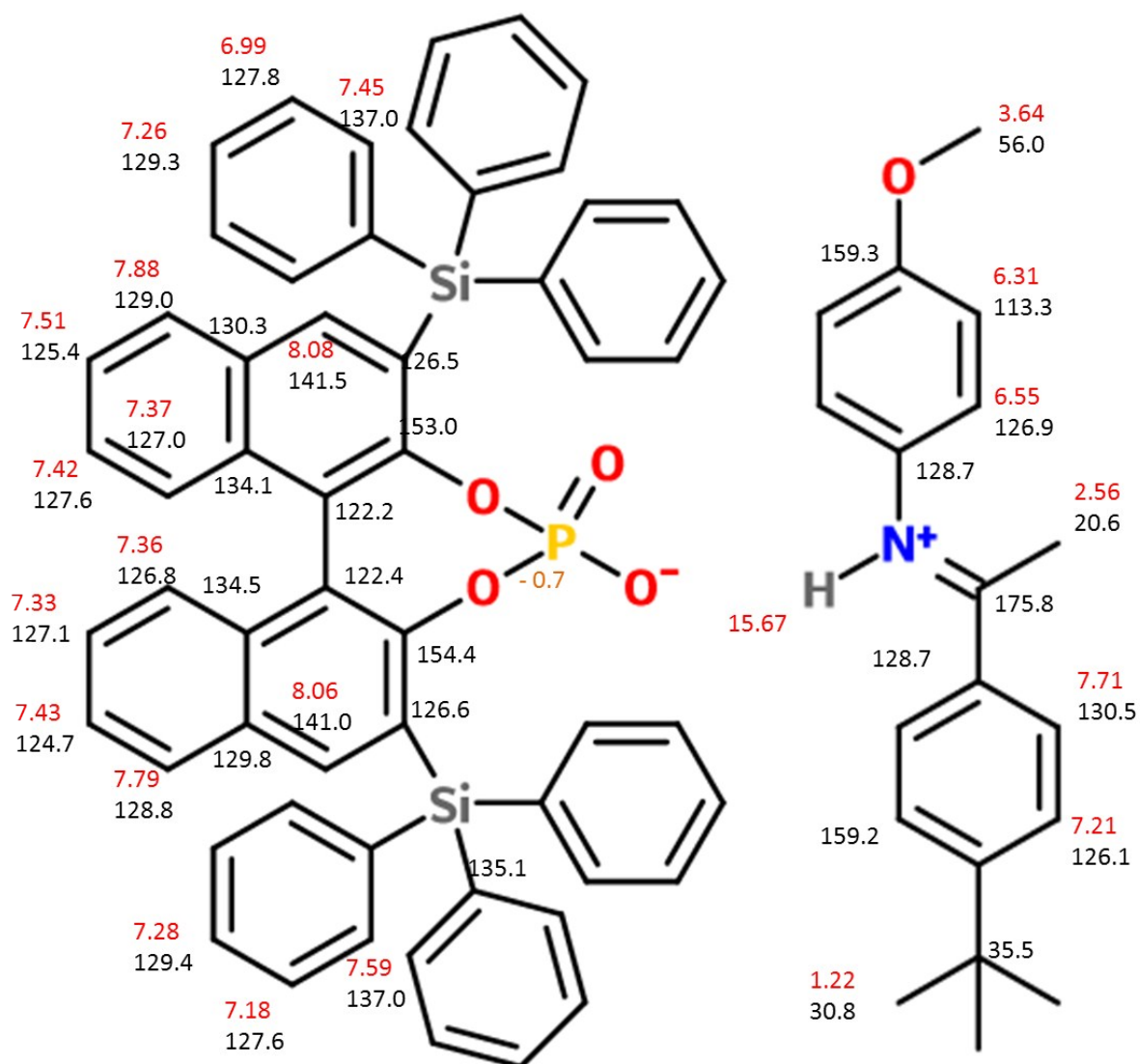
S8. Complex (TiPSY/2E)



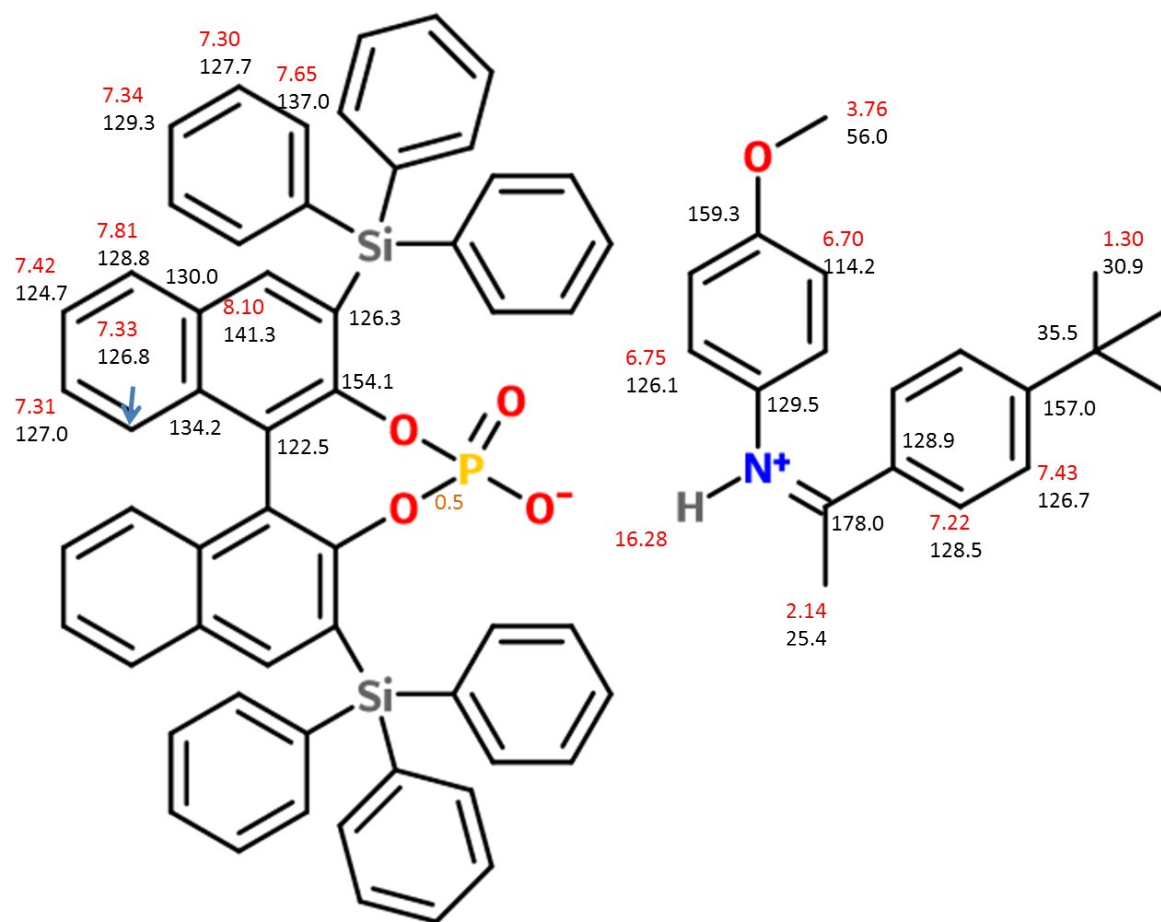
S9. Complex (TiPSY/2Z)



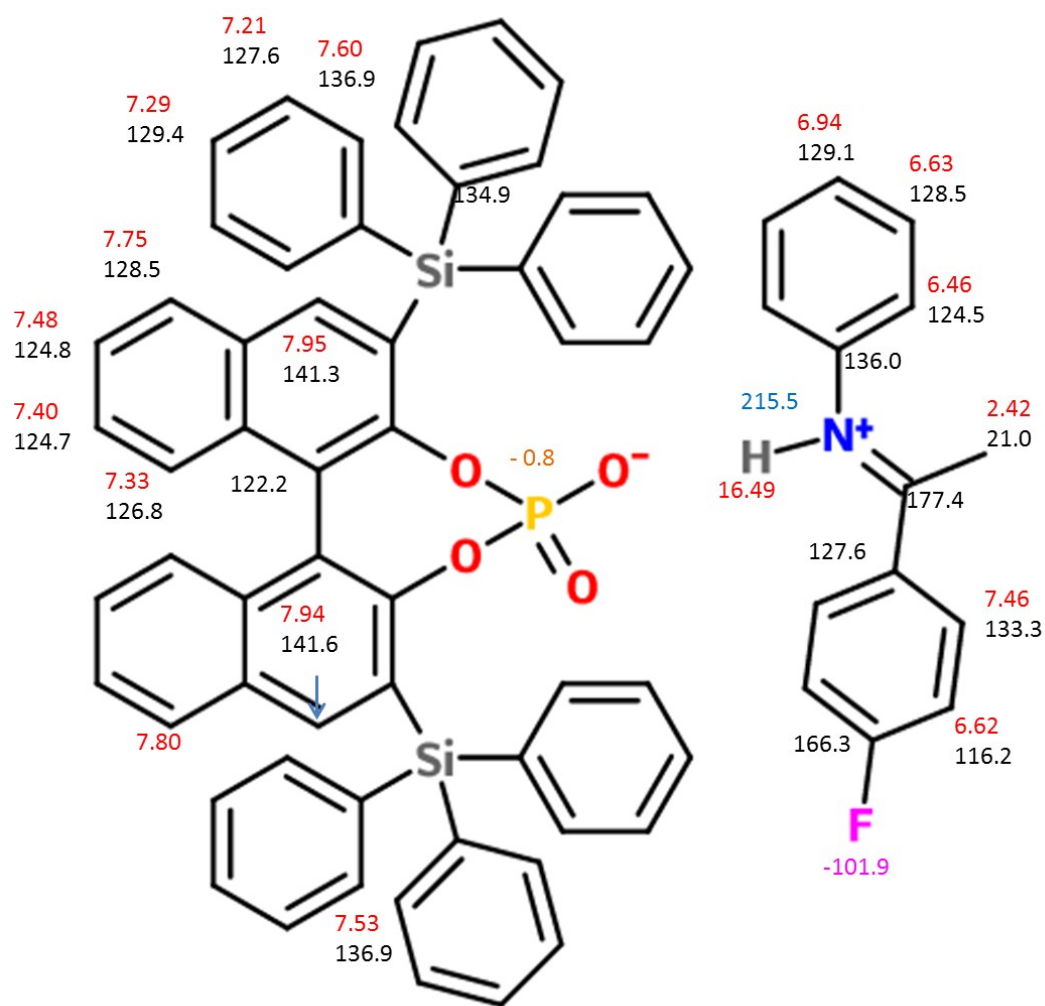
S10. Complex (TiPSY/3E)



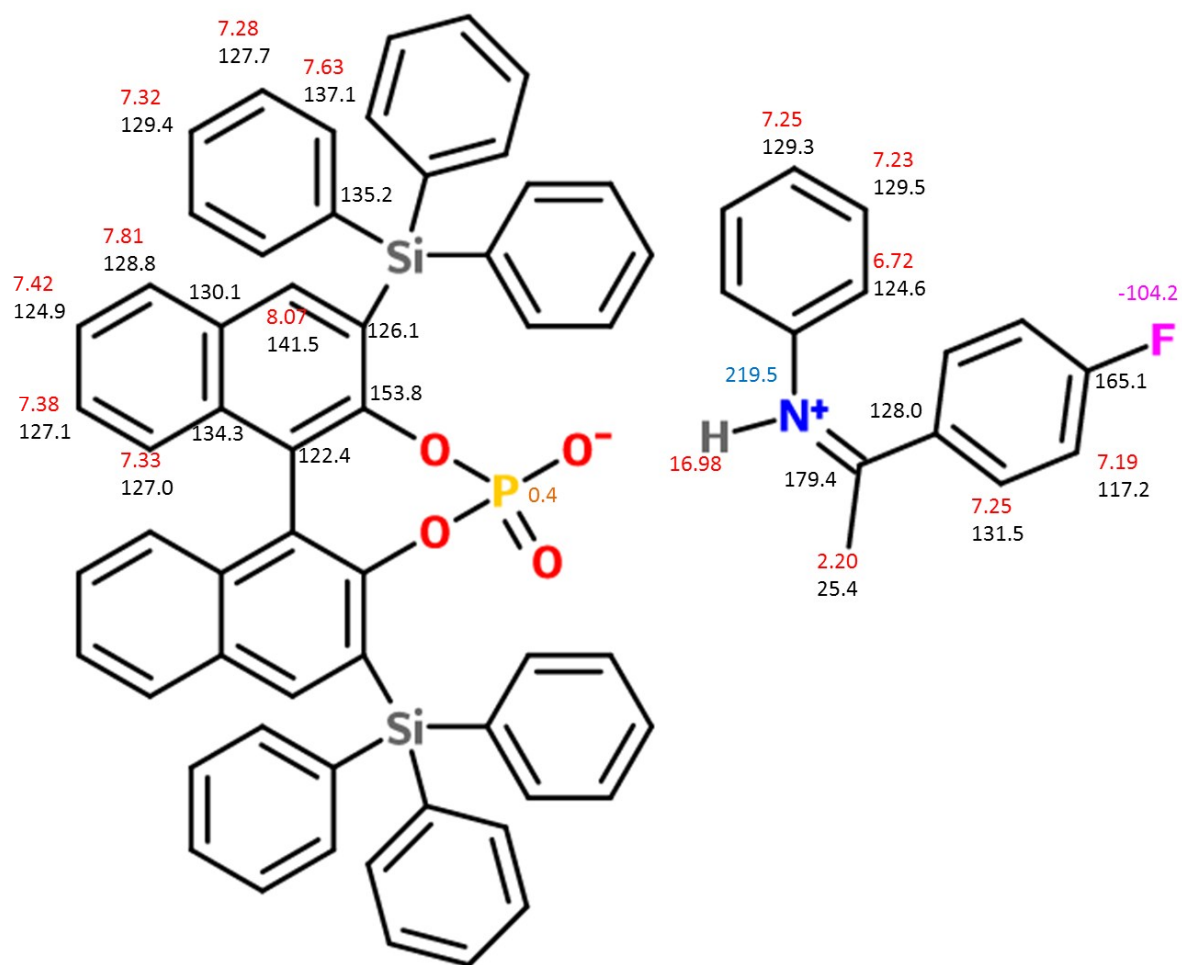
S11. Complex (TiPSY/3Z)



S12. Complex (TiPSY/4E)

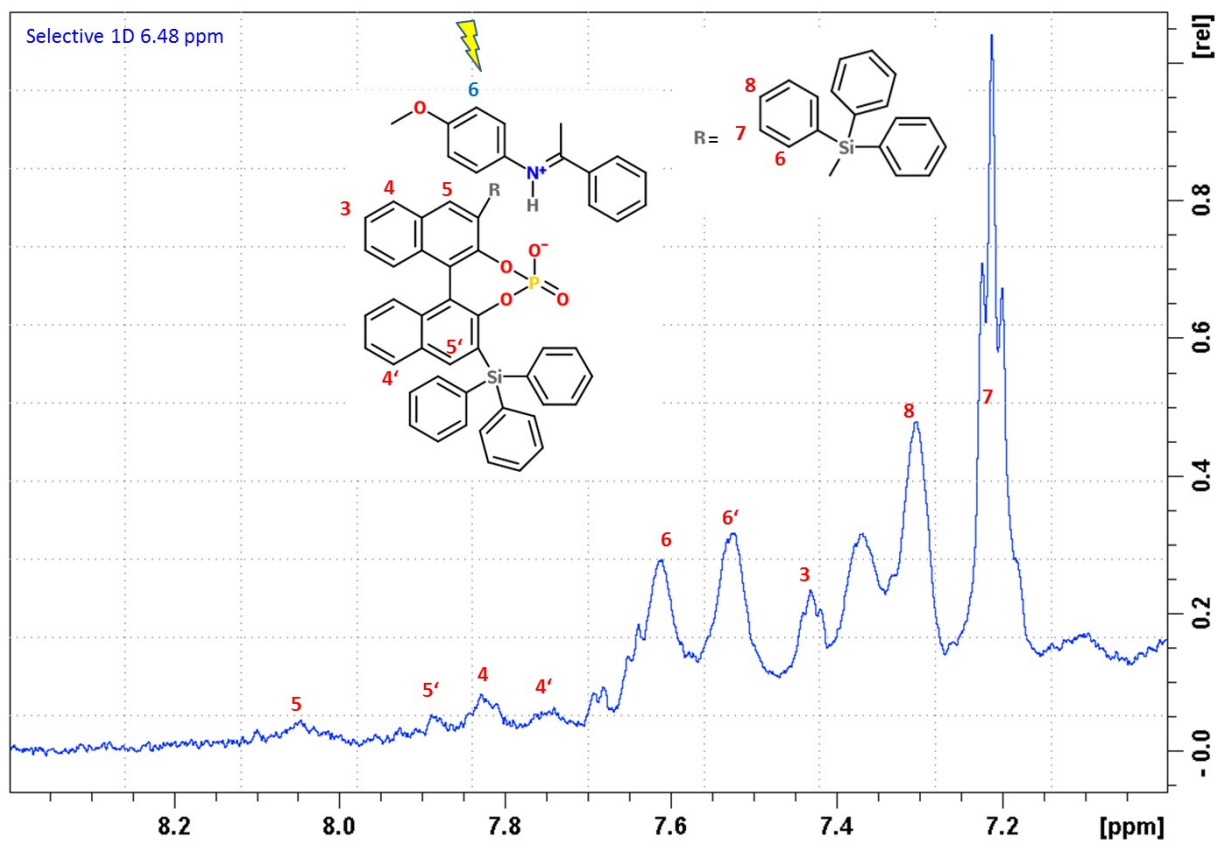


S13. Complex (TiPSY/4Z)



Structure identification of all TiPSY/*E*-imine complexes

S14. Type II TiPSY/1E Complex



From imine **2**, five NOEs to the catalyst backbone signals were observed (spins 3, 4, 4', 5 and 5').

Experiment parameters:

Pulse sequence: selnoggp,

Mixing time 100 ms,

Selective 180° Gaussian pulse at 6.48 ppm: 19 ms using Topspin shape tool.

Time domain: 64k points,

Spectral window 22 ppm,

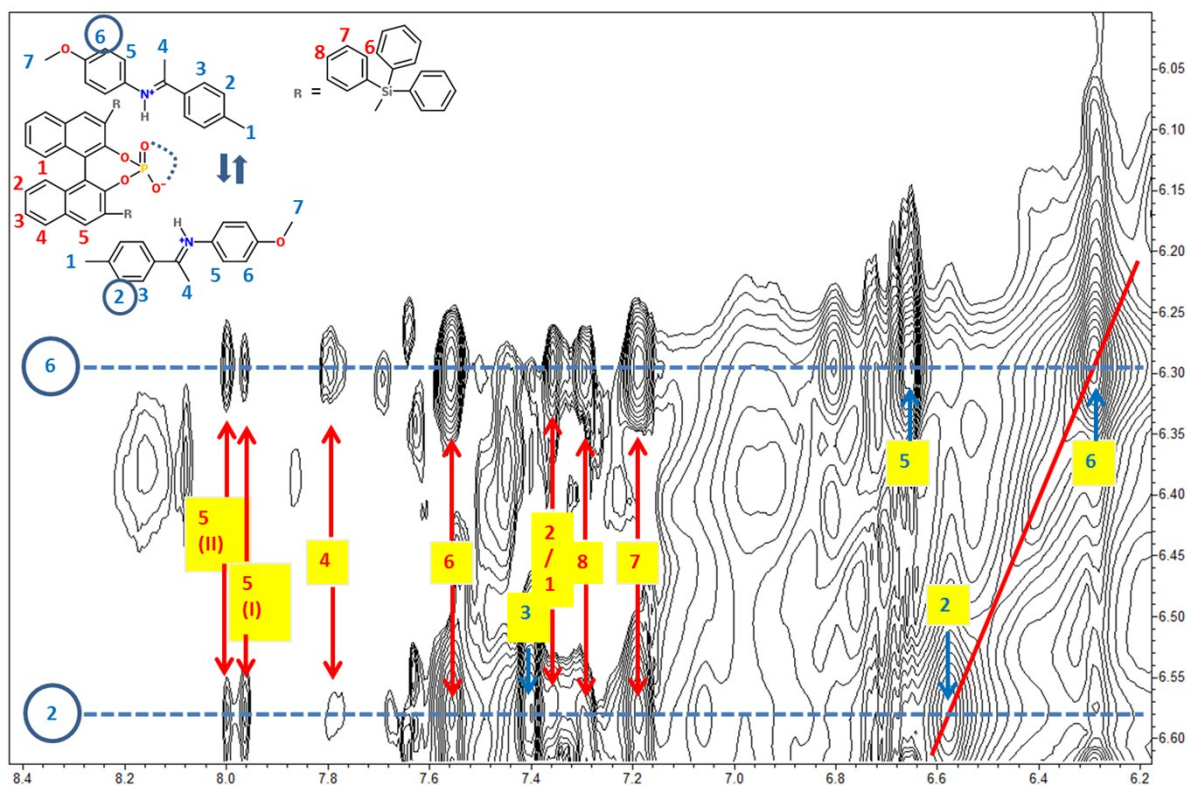
¹H offset frequency: 10 ppm,

Recycling delay: 4s,

Number of scans: 1k.

Experiment time: 1h54min.

S15. Types I - II TiPSY/2E Complex

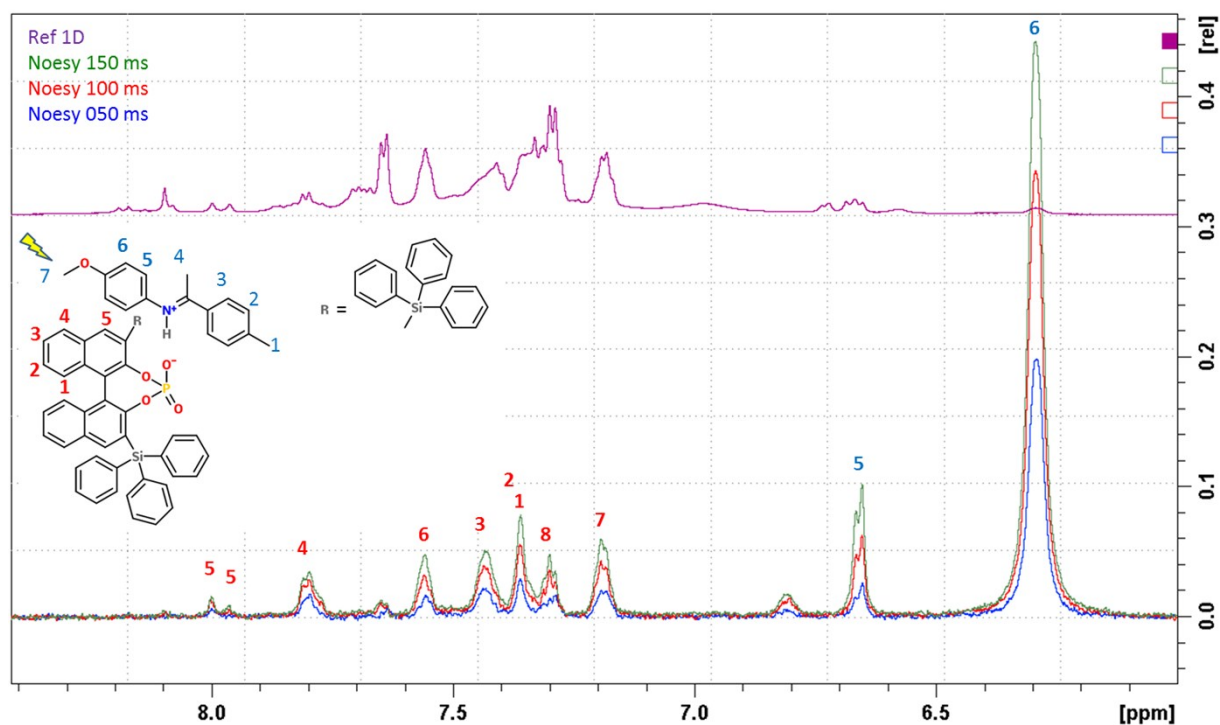


With imine **15**, from two different examples, intermolecular NOEs were found to TiPSY backbone signals (spins 1 or 2 in overlap, 3, 4, 5 and 5'). Here both patterns between *Type I* and *Type II* can be directly compared.

Experiment parameters:

Pulse sequence: noesygpphpp,
 Mixing time 200 ms,
 Time domain: 8k x 512 points,
 Spectral window 34 x 11.5 ppm (folded indirect dimension)
¹H offset frequency: 3.75 ppm,
 Recycling delay: 2s,
 Number of scans: 32.
 Experiment time: 11h12min.

S16. Type II TiPSY/2E Complex



With the imine **3**, from two different examples, intermolecular NOEs were found with TiPSY backbone signals (spins 1 or 2 in overlap, 3, 4, 5 and 5'). The same pattern is found with a selective excitation on the methoxy group.

Experiment parameters:

Pulse sequence: selnoggp.

Mixing time 50 - 150 ms.

Selective 180° Gaussian pulse at 3.66 ppm: 78 ms using Topspin shape tool.

Time domain: 64k points.

Spectral window 22 ppm.

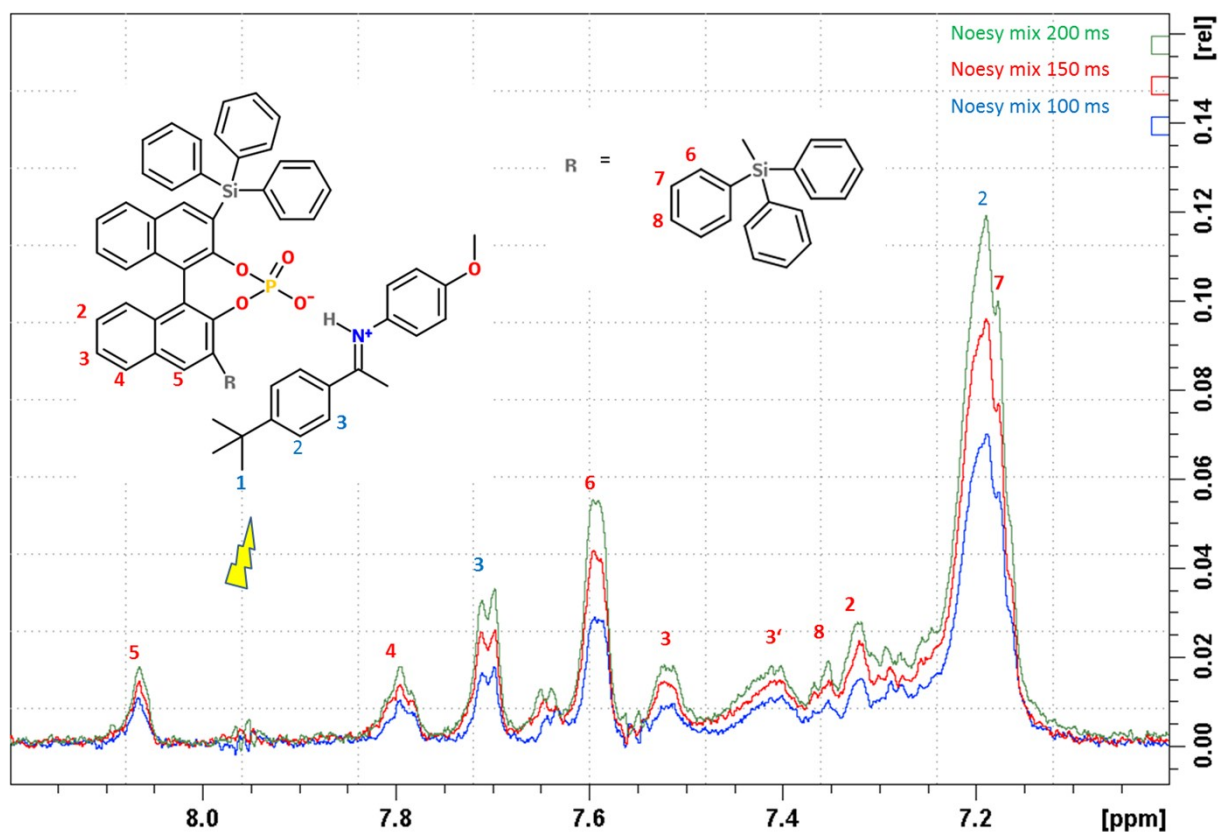
1H offset frequency: 9 ppm.

Recycling delay: 4s.

Number of scans: 1k.

Experiment time: 1h54min.

S17. Type I TiPSY/3E Complex



Experiment parameters:

Pulse sequence: selnogg,

Mixing time 100 - 300 ms,

Selective 180° Gaussian pulse at 1.22 ppm: 72 ms using Topspin shape tool.

Time domain: 64k points,

Spectral window 22 ppm,

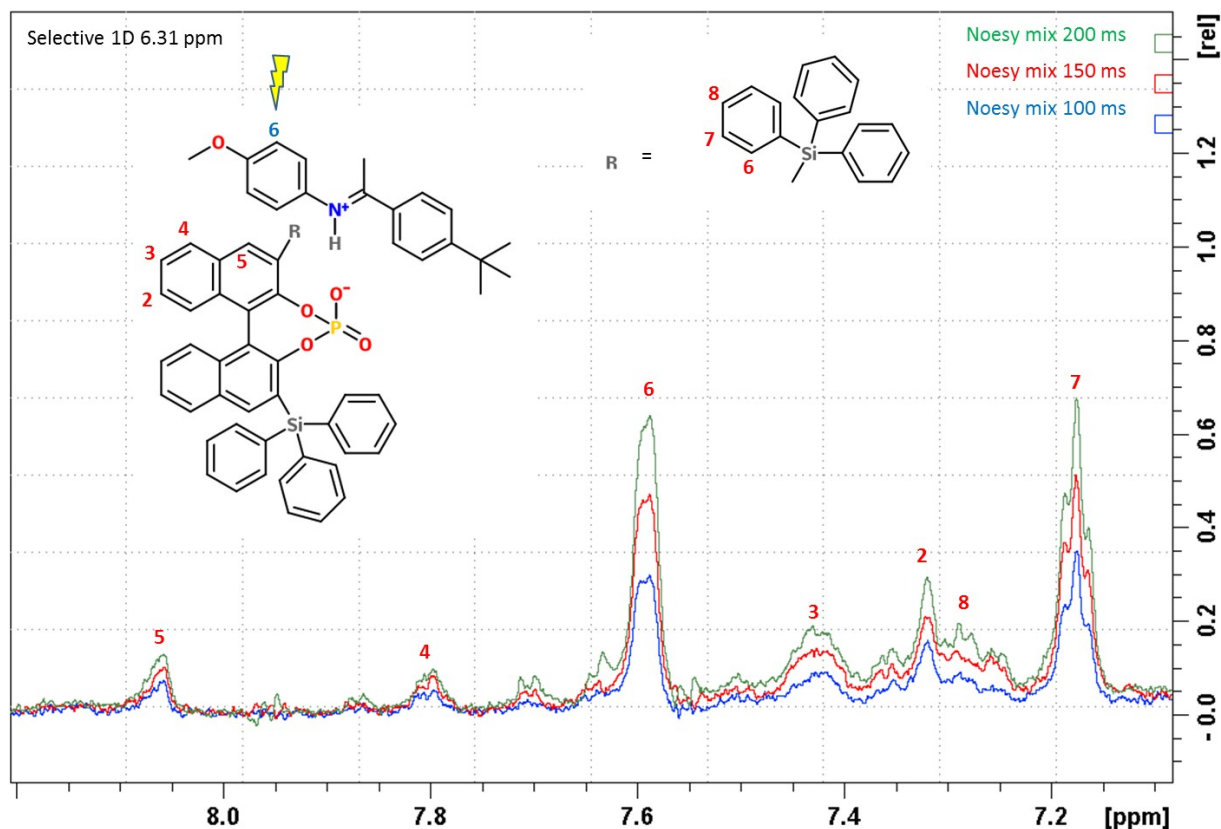
¹H offset frequency: 10 ppm,

Recycling delay: 4s,

Number of scans: 1k.

Experiment time: 1h54min.

S18. Type II TiPSY/3E Complex



From imine **4**, four specific intermolecular NOE with TiPSY backbone were detected (spins 2, 3, 4 and 5).

Experiment parameters:

Pulse sequence: selnoggp,

Mixing time 100; 150; 200 ms,

Selective 180° Gaussian pulse at 6.31 ppm: 20 ms using Topspin shape tool.

Time domain: 64k points,

Spectral window 22 ppm,

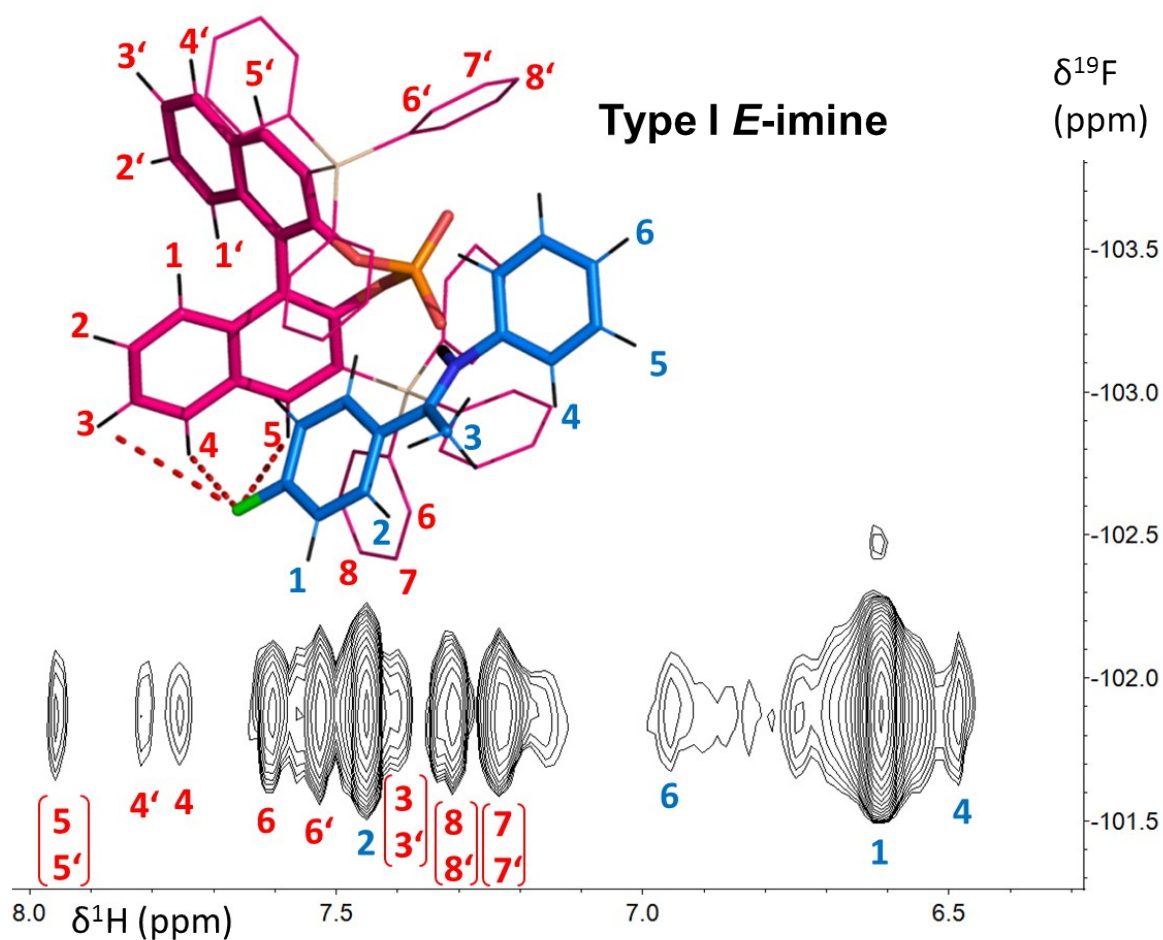
¹H offset frequency: 10 ppm,

Recycling delay: 5s,

Number of scans: 1k.

Experiment time: 1h54min.

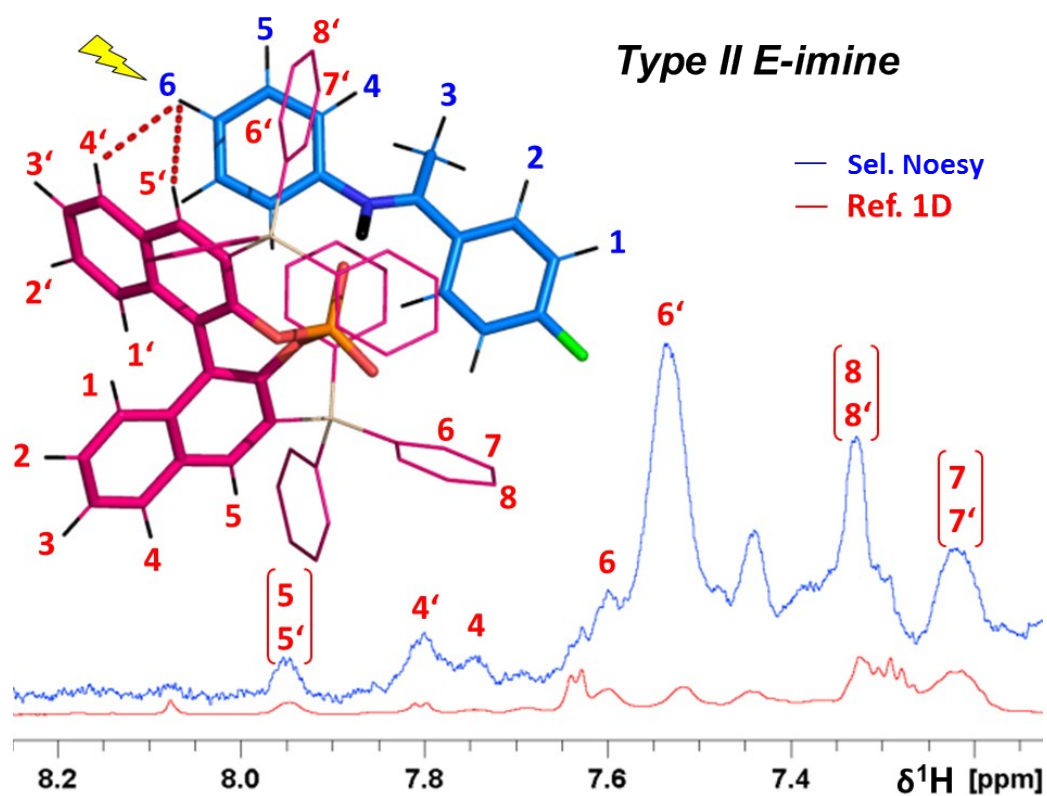
S19. Type I TiPSY/4E Complex



Experiment parameters:

Pulse sequence: hoesyph,
 Mixing time 300 ms,
 Time domain: 4k x 32 points,
 Spectral window 26 x 6 ppm,
 ^1H offset frequency: 10 ppm,
 ^{19}F offset frequency -103 ppm,
 Recycling delay: 2s,
 Number of scans: 32.
 Experiment time: 1h24min.

S20. Type II TiPSY/4E Complex



Experiment parameters:

Pulse sequence: selnoggp,

Mixing time 100 ms,

Selective 180° Gaussian pulse at 6.94 ppm: 49 ms using Topspin shape tool.

Time domain: 64k points,

Spectral window 22 ppm,

^1H offset frequency: 10 ppm,

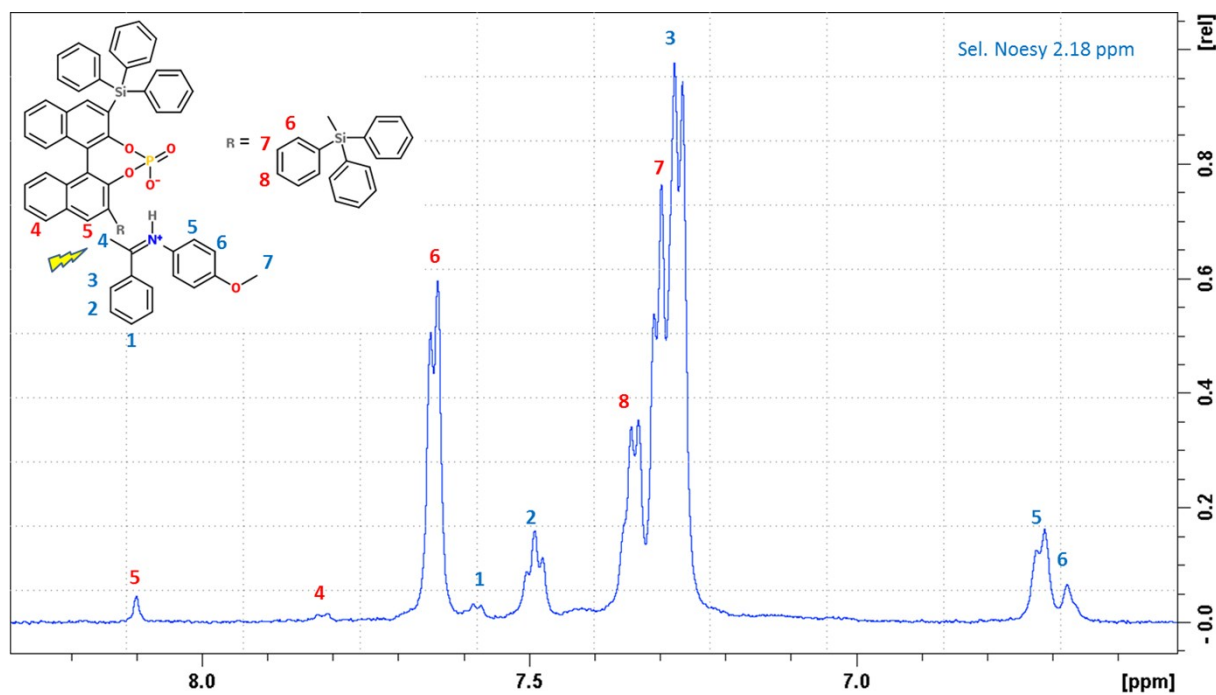
Recycling delay: 4s,

Number of scans: 1k.

Experiment time: 1h54min.

Structure identification of all TiPSY/Z-imine complexes

S21. Type I TiPSY/1Z Complex



Experiment parameters:

Pulse sequence: selnoggp,

Mixing time 200 ms,

Selective 180° Gaussian pulse at 2.18 ppm: 89 ms using Topspin shape tool.

Time domain: 64k points,

Spectral window 22 ppm,

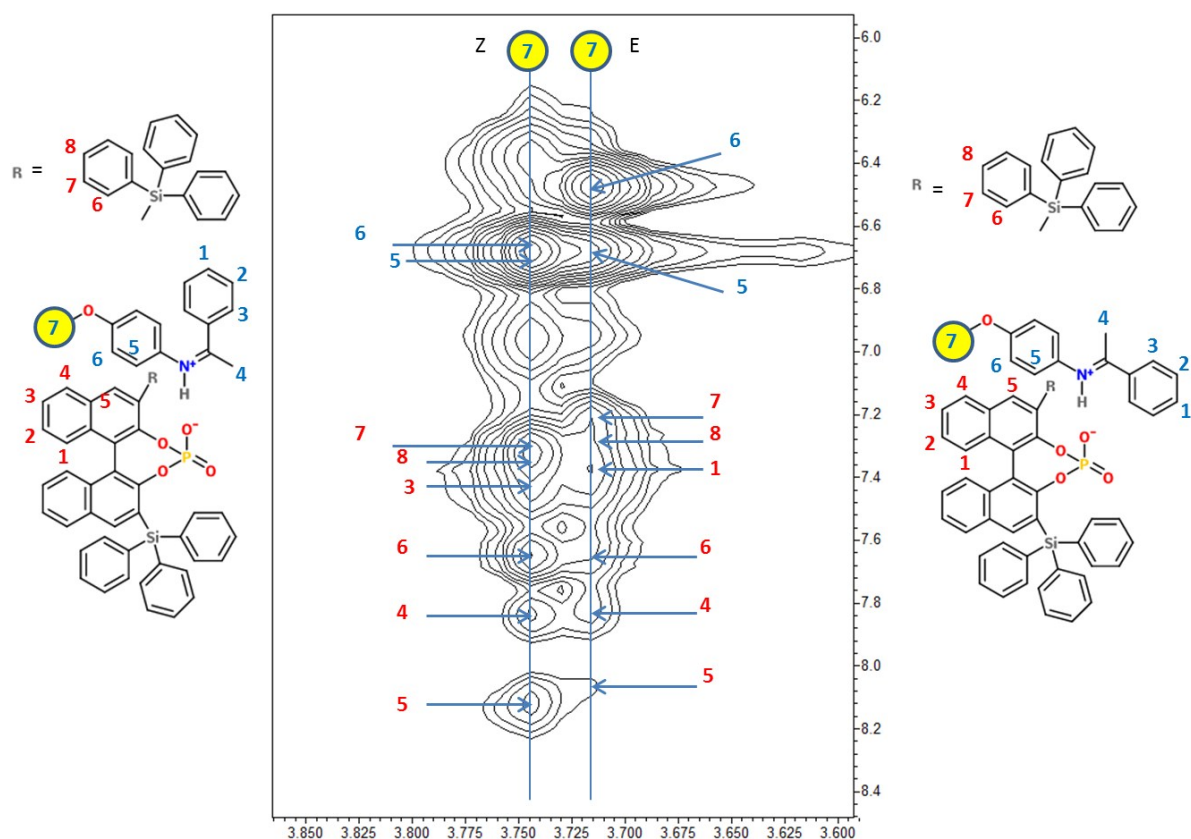
¹H offset frequency: 10 ppm,

Recycling delay: 4s,

Number of scans: 1k.

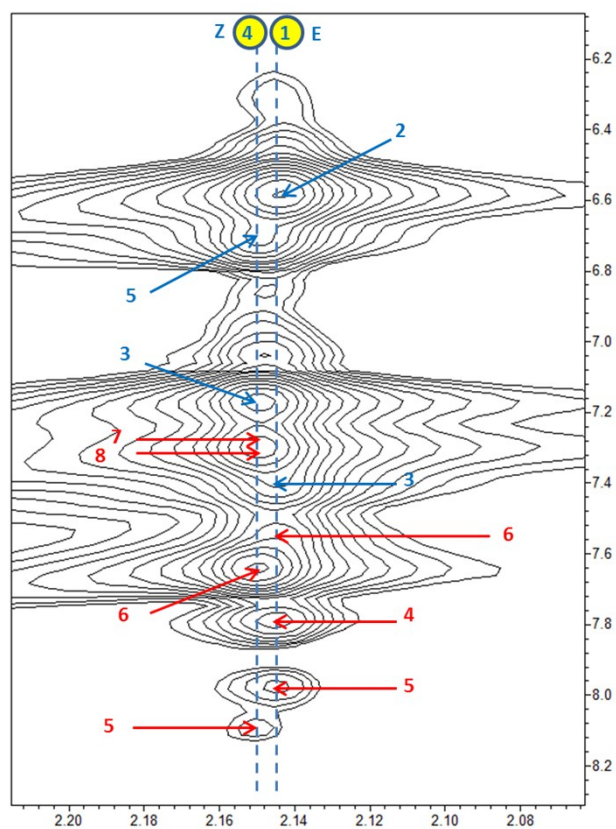
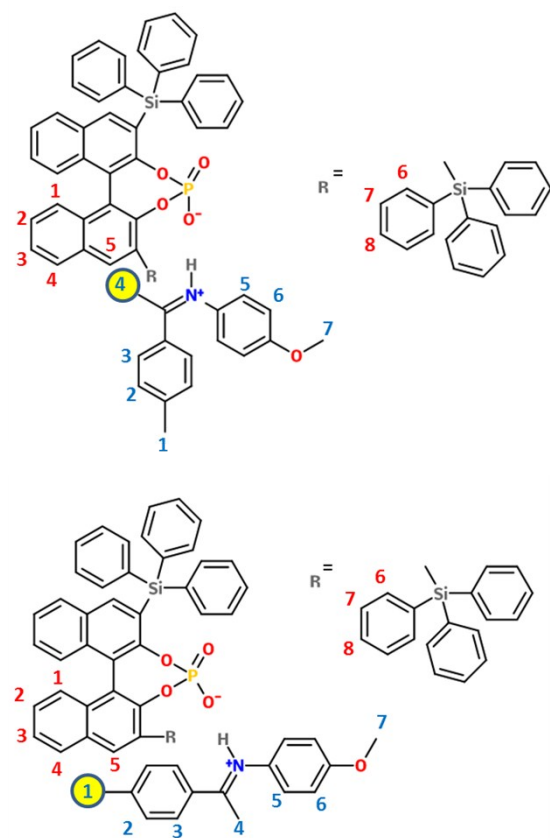
Experiment time: 1h56min.

S22. Type II TiPSY/1E-Z Complexes



Pulse sequence: noesygpphpp,
 Mixing time 500 ms,
 Time domain: 4k x 256 points,
 Spectral window 29 x 13 ppm (folded indirect dimension)
¹H offset frequency: 5.5 ppm,
 Recycling delay: 2s,
 Number of scans: 32.
 Experiment time: 6h4min.

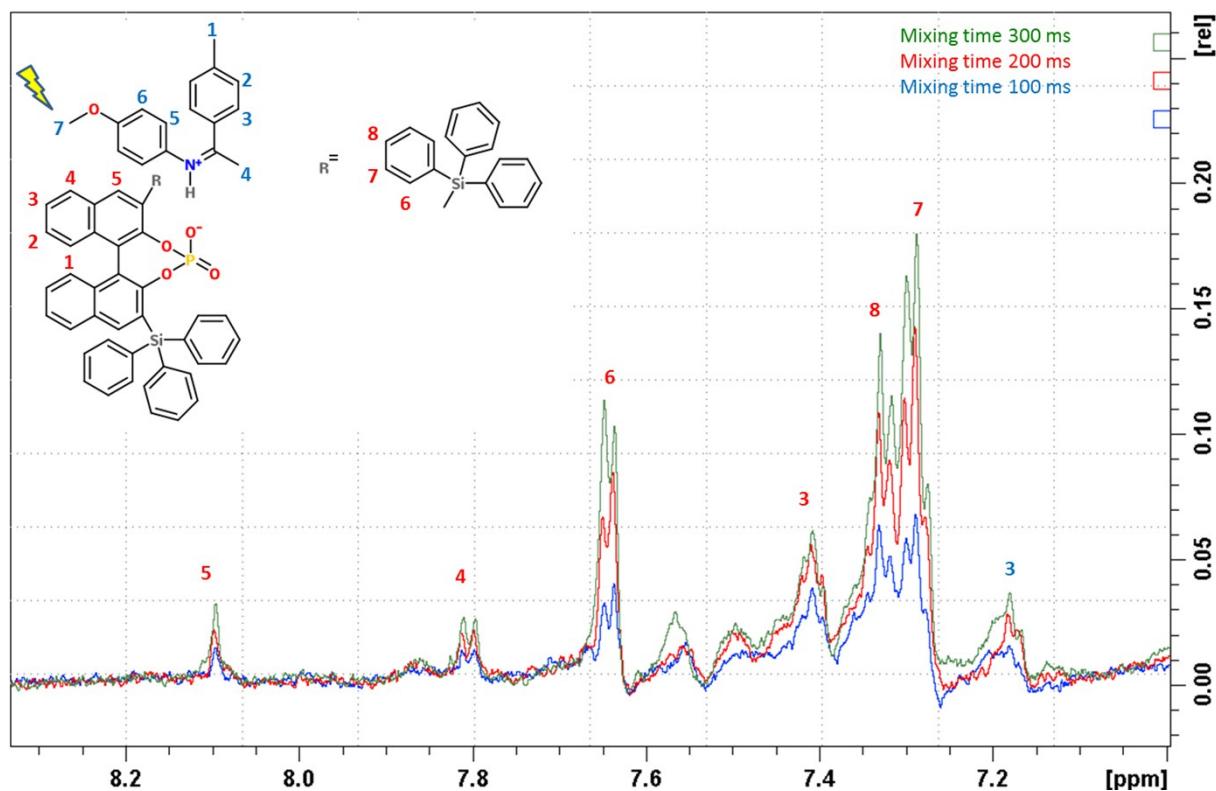
S23. Type I TiPSY/2E-Z Complexes



Experiment parameters:

Pulse sequence: noesygpphpp,
 Mixing time 200 ms,
 Time domain: 4k x 512 points,
 Spectral window 22 x 22 ppm
¹H offset frequency: 9 ppm,
 Recycling delay: 2s,
 Number of scans: 32.
 Experiment time: 10h56min.

S24. Type II TiPSY/2Z Complex



Experiment parameters:

Pulse sequence: selnoggps,

Mixing time 100, 200 and 300 ms,

Selective 180° Gaussian pulse at 3.75 ppm: 69 ms using Topspin shape tool.

Time domain: 24k points,

Spectral window 22 ppm,

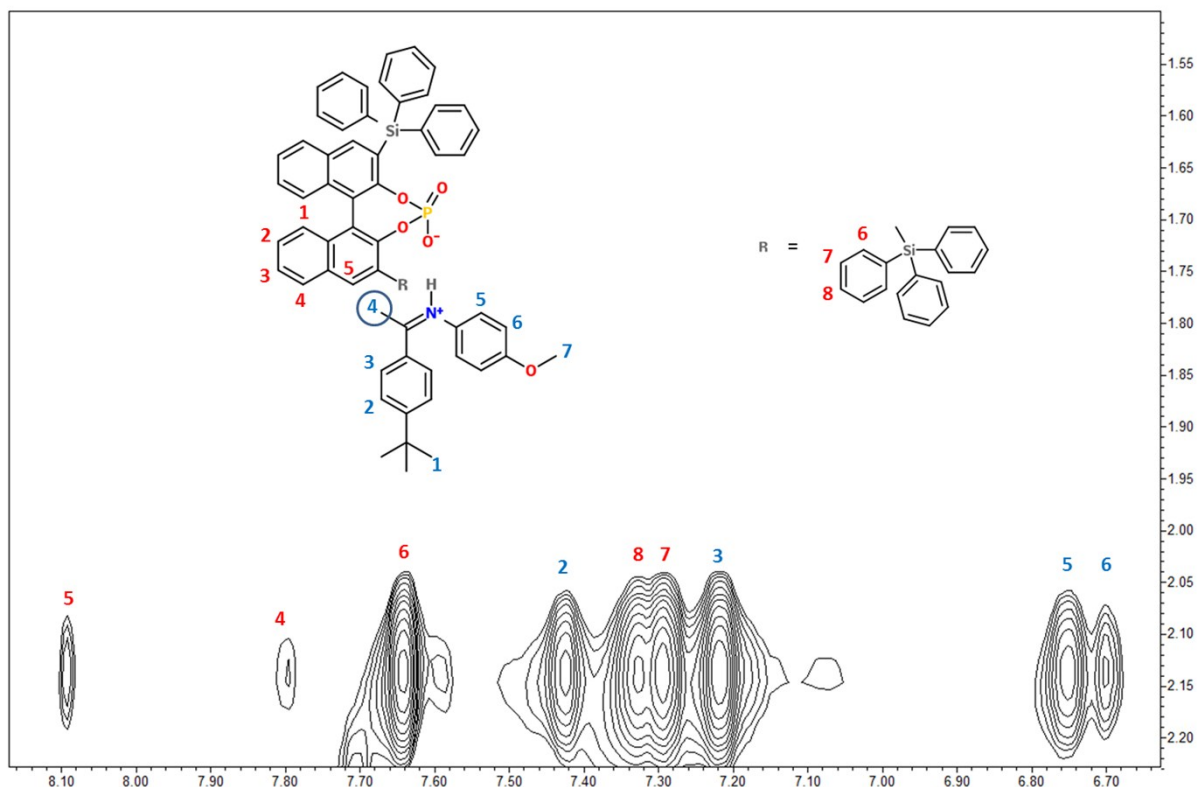
^1H offset frequency: 9 ppm,

Recycling delay: 8s,

Number of scans: 768.

Experiment time: 1h57min.

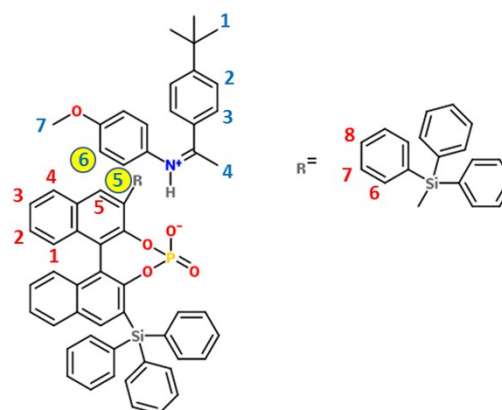
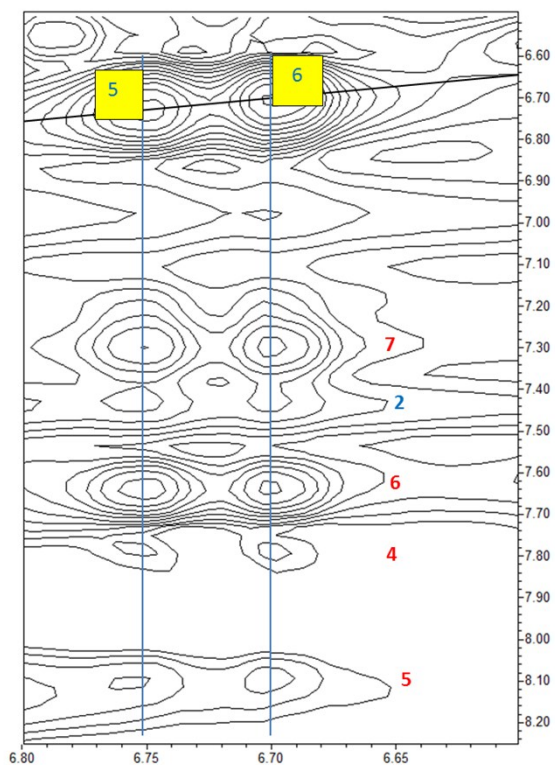
S25. Type I TiPSY/3Z Complex



Experiment parameters:

Pulse sequence: noesygpphp,
 Mixing time 300 ms,
 Time domain: 4k x 512 points,
 Spectral window 22 x 22 ppm
¹H offset frequency: 10 ppm,
 Recycling delay: 2s,
 Number of scans: 40.
 Experiment time: 11h12min.

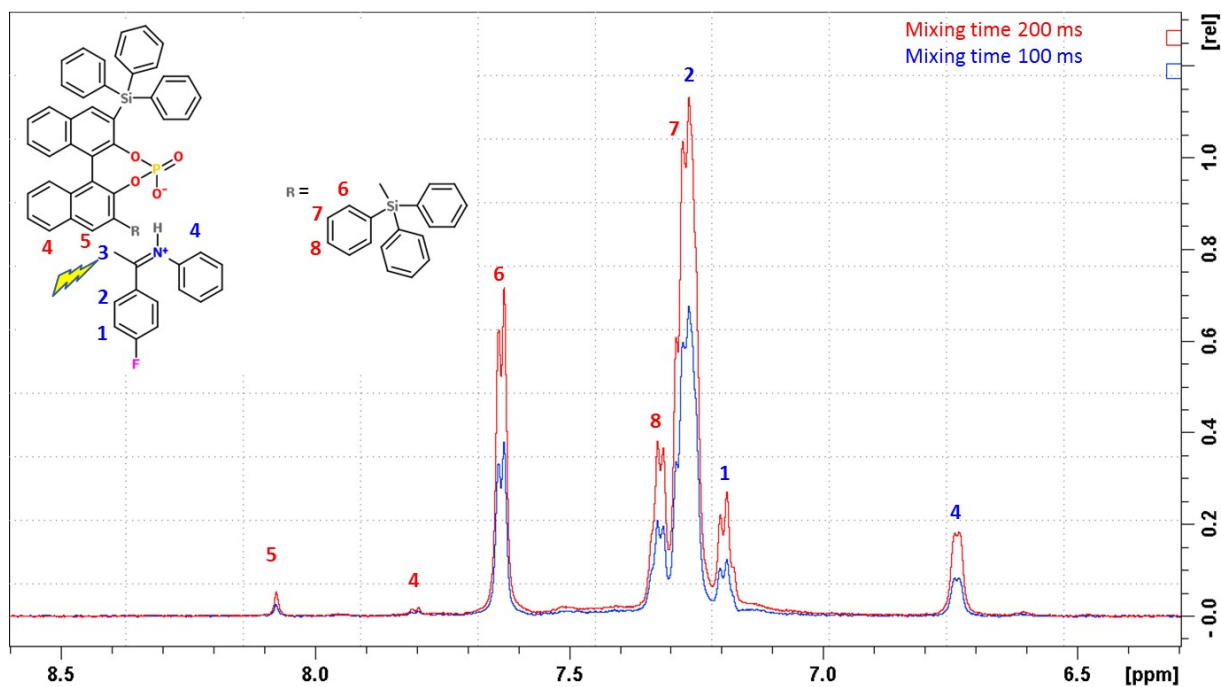
S26. Type II TiPSY/3Z Complex



Experiment parameters:

Pulse sequence: noesygpphpp,
 Mixing time 300 ms,
 Time domain: 4k x 512 points,
 Spectral window 22 x 22 ppm
¹H offset frequency: 10 ppm,
 Recycling delay: 2s,
 Number of scans: 40.
 Experiment time: 11h12min.

S27. Type I TiPSY/4Z Complex



Experiment parameters:

Pulse sequence: selnpgp.

Mixing time 100 - 200 ms.

Selective 180° Gaussian pulse at 3.66 ppm: 38 ms using Topspin shape tool.

Time domain: 64k points.

Spectral window 22 ppm.

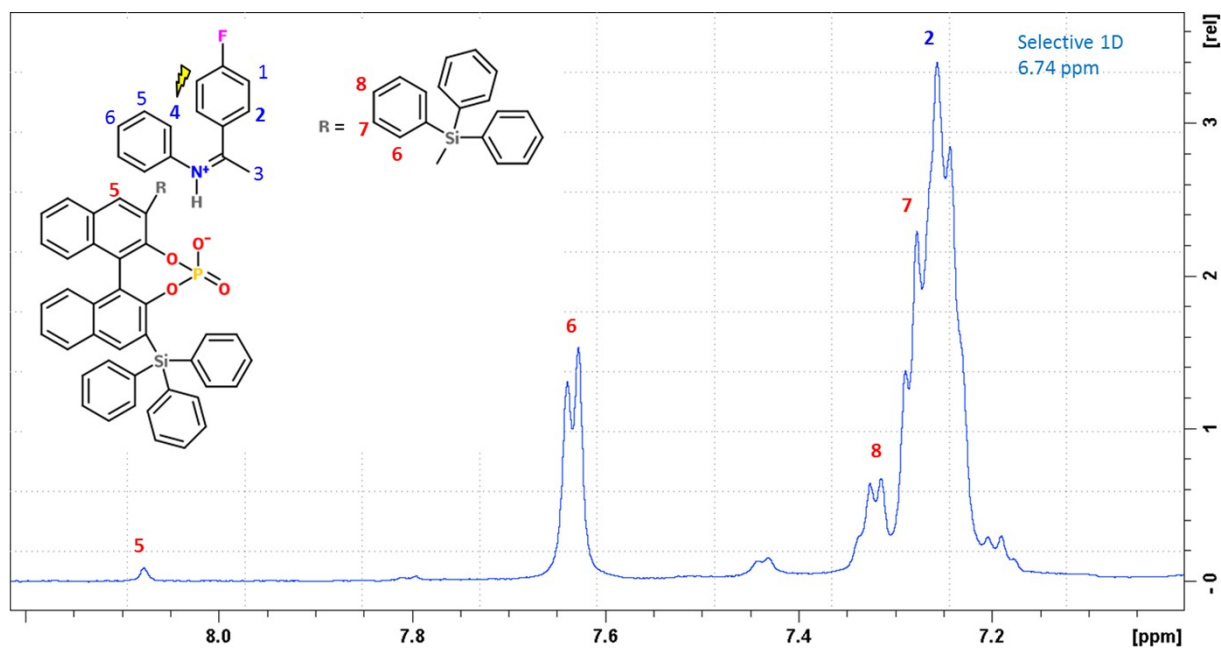
1H offset frequency: 10 ppm.

Recycling delay: 4s.

Number of scans: 1k.

Experiment time: 1h55min.

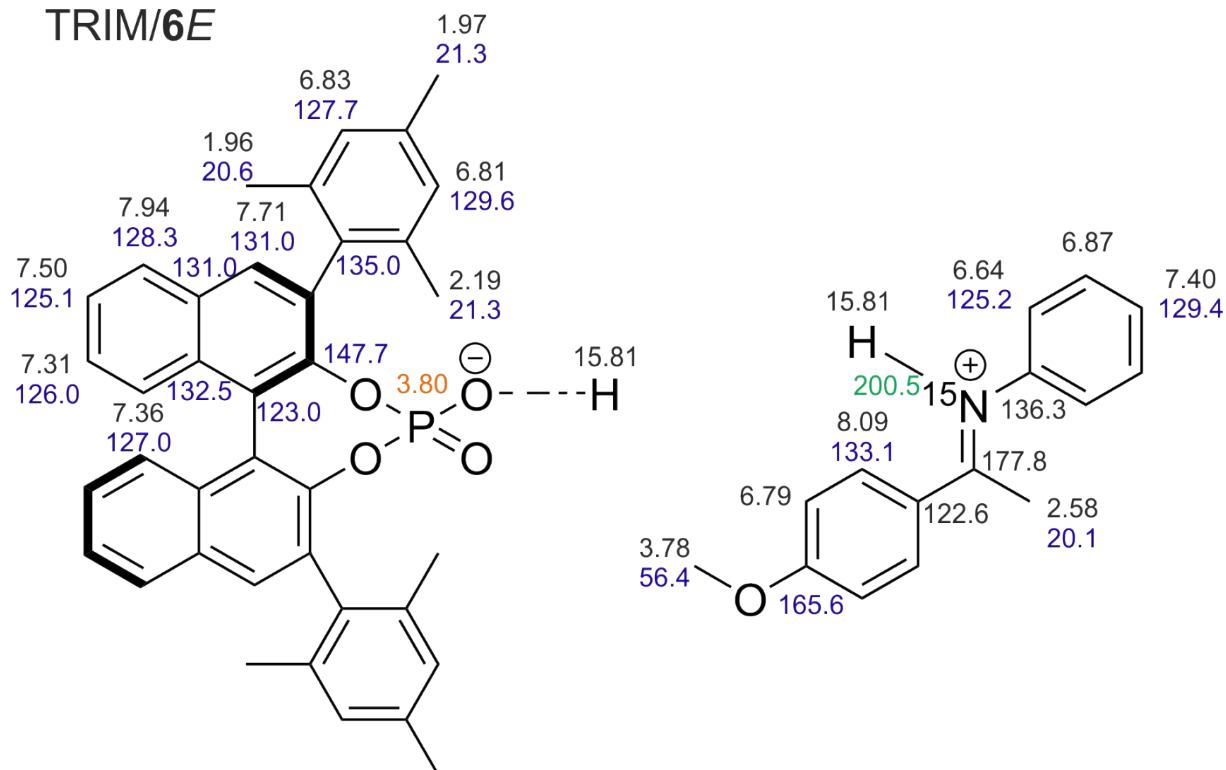
S28. Type II TiPSY/4Z Complex



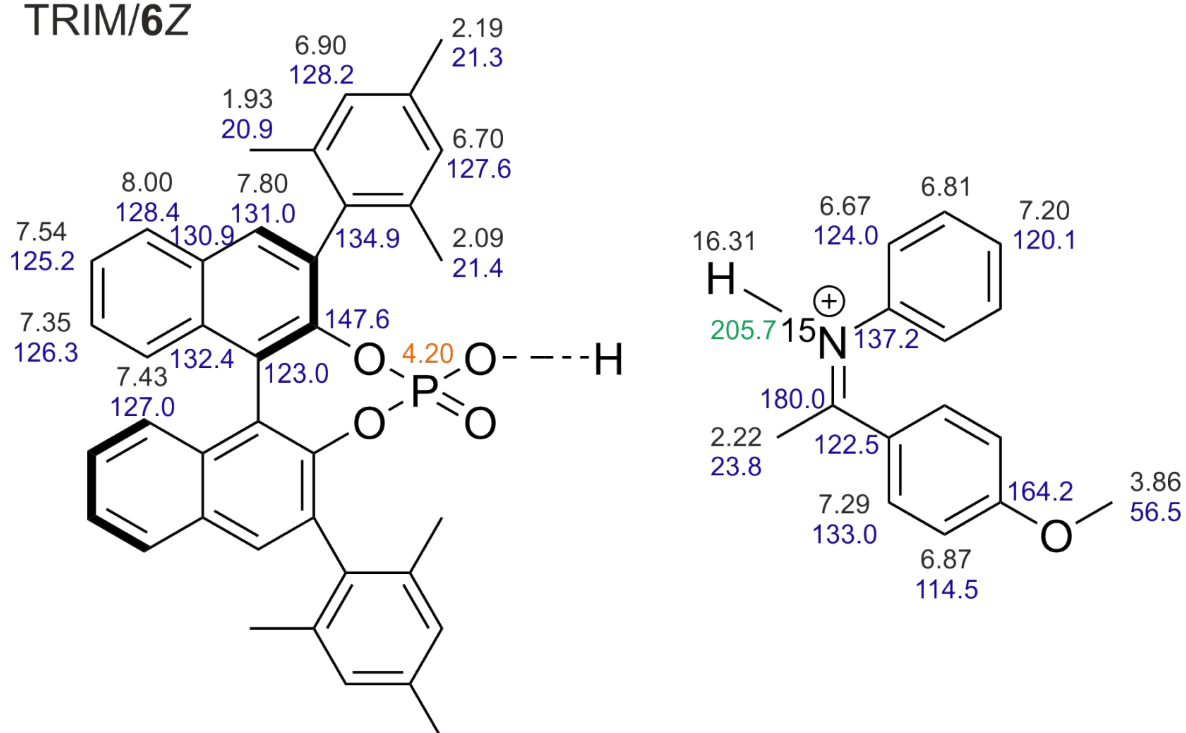
S30. Complexes (TRIM/6)

Colour code: blue – ^1H / black – ^{13}C / green – ^{15}N / orange – ^{31}P

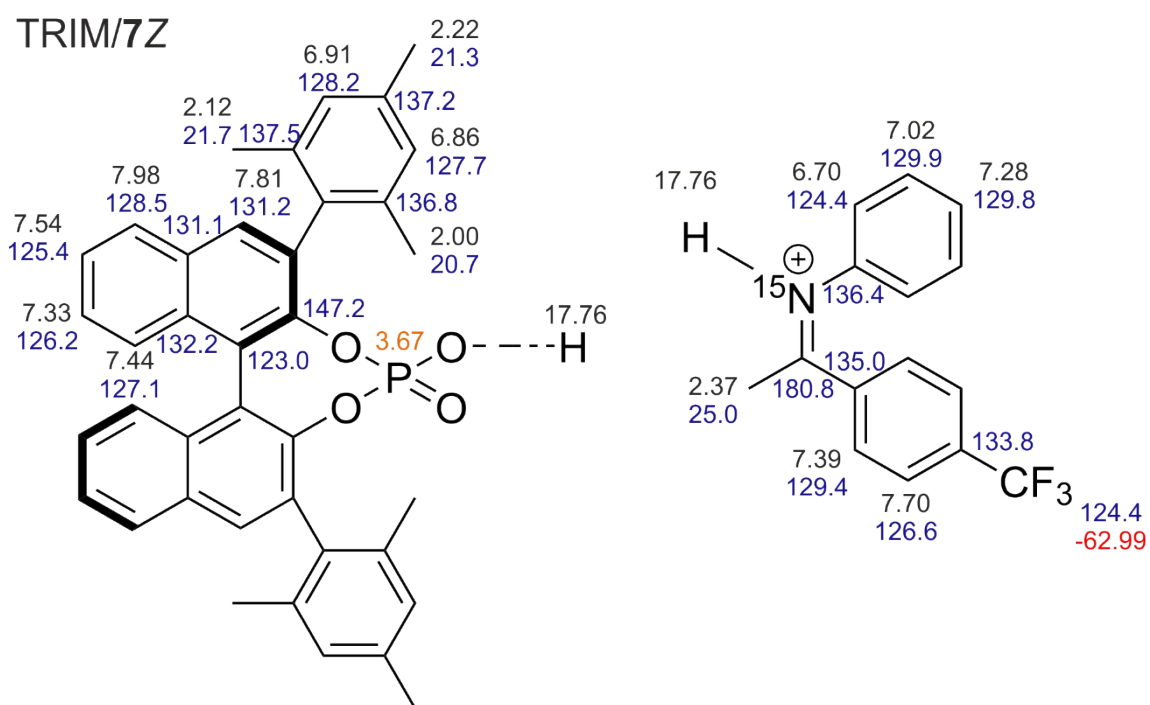
TRIM/6E



TRIM/6Z

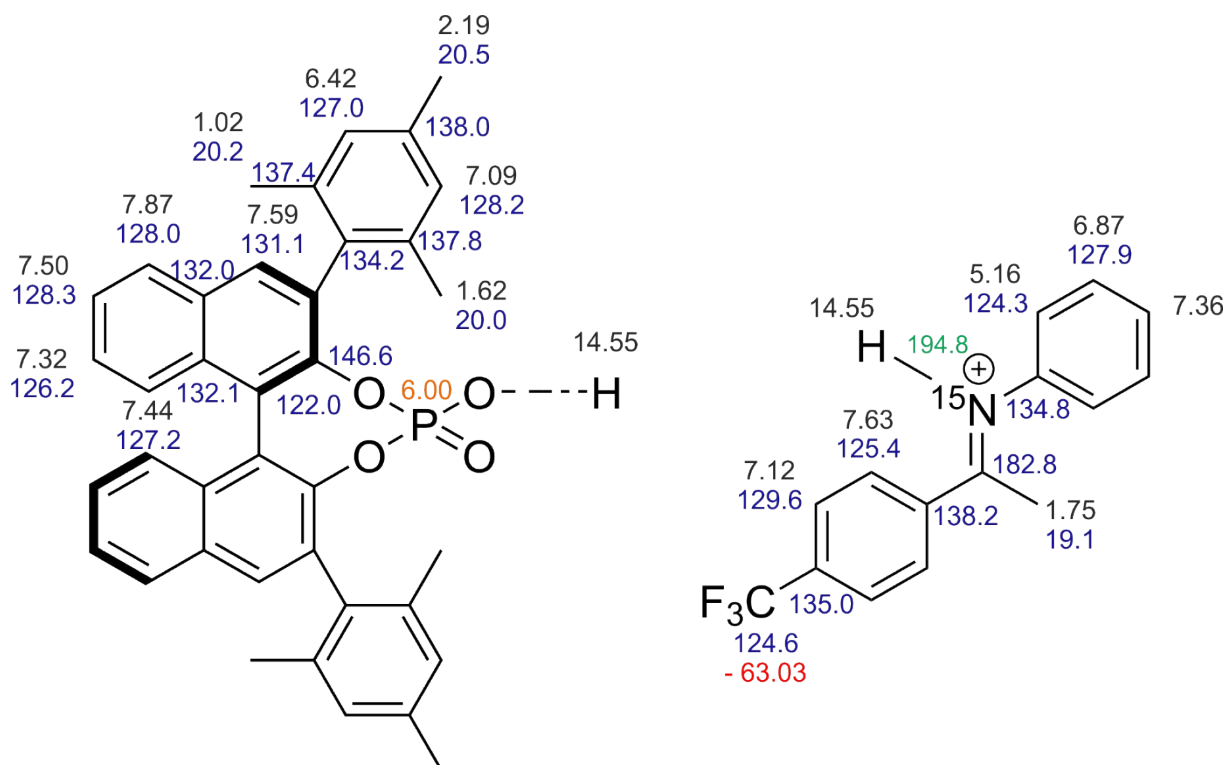


Colour code: blue – ^1H / black – ^{13}C / green – ^{15}N / orange – ^{31}P / red – ^{19}F



S32. Complexes [TRIM/7E]₂

Colour code: blue – ¹H / black – ¹³C / green – ¹⁵N / orange – ³¹P / red – ¹⁹F



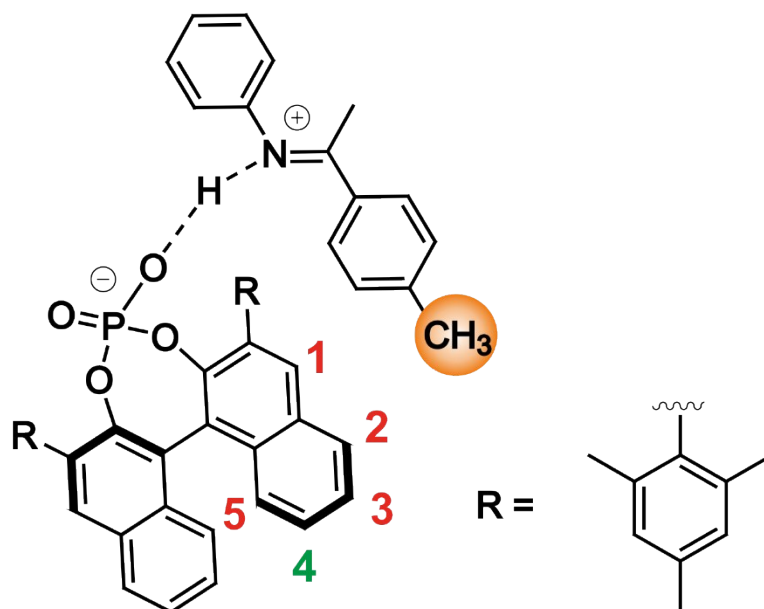
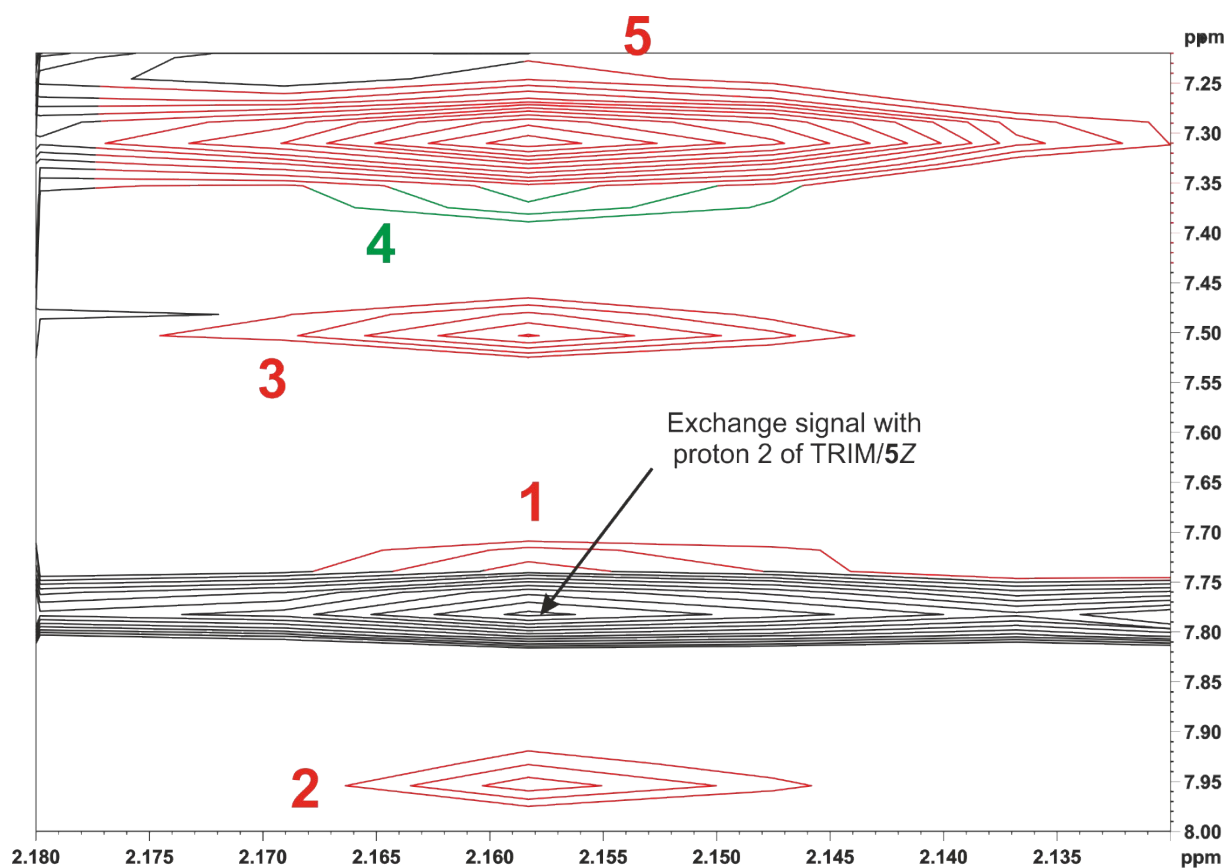
Structure identification of all TRIM/imine complexes

Experimental parameters

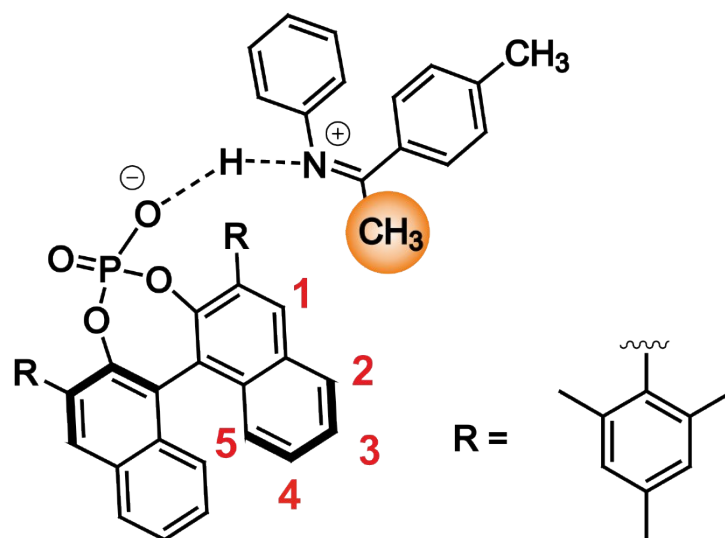
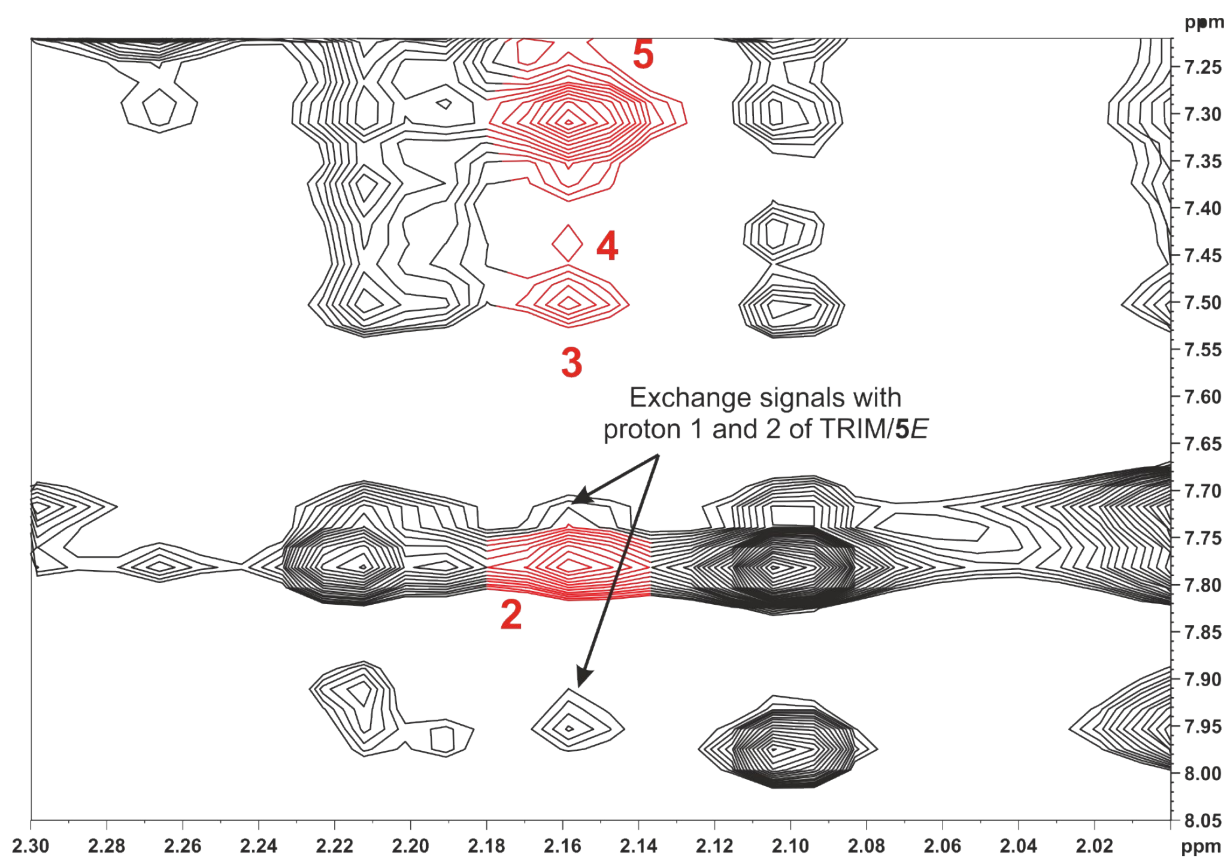
Pulse sequence: hoesyph
Mixing time 350 ms,
Time domain: 4k x 1250 points,
Spectral window 6 x 22 ppm,
¹H offset frequency: 10 ppm,
¹⁹F offset frequency -63 ppm,
Recycling delay: 2s,
Number of scans: 8.
Experiment time: 16h38min.
Sample concentration: 100 mM

Pulse sequence: noesygpphp,
Mixing time 300 ms,
Time domain: 4k x 512-1024 points,
Spectral window 22 x 22 ppm
¹H offset frequency: 10 ppm,
Recycling delay: 2s,
Number of scans: 8-16.
Experiment time: 12h29min.
Sample concentration: 50-100 mM

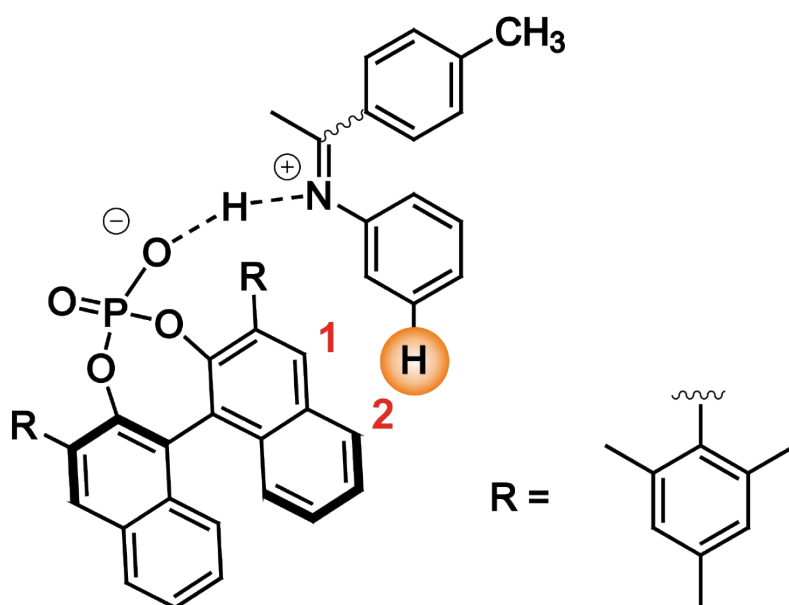
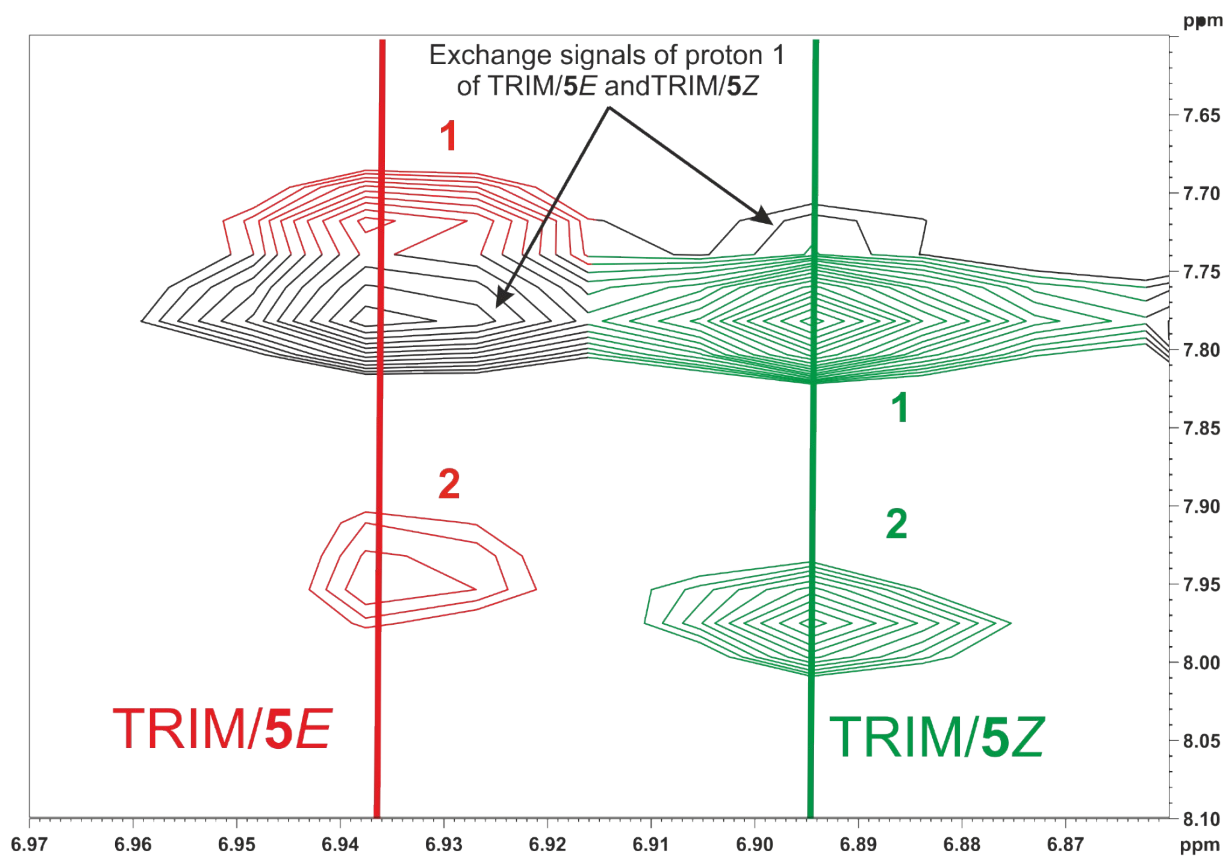
S33. Type I TRIM/5E Complex



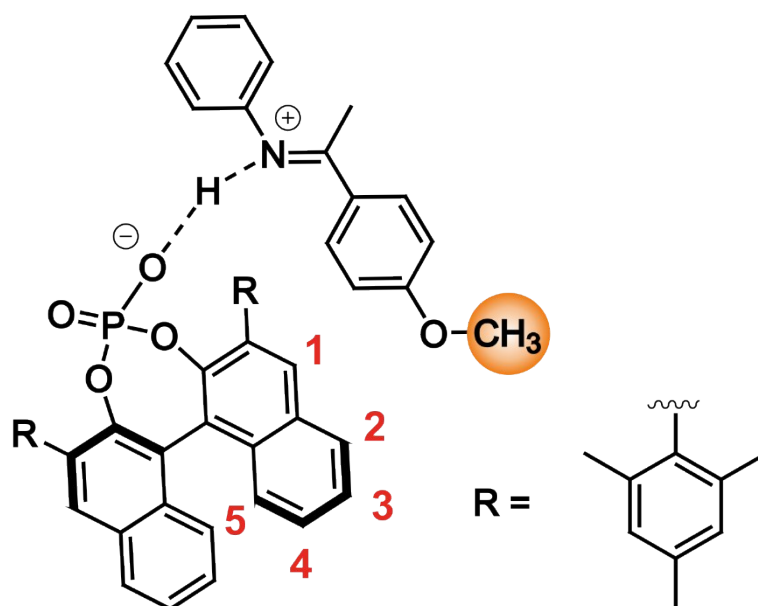
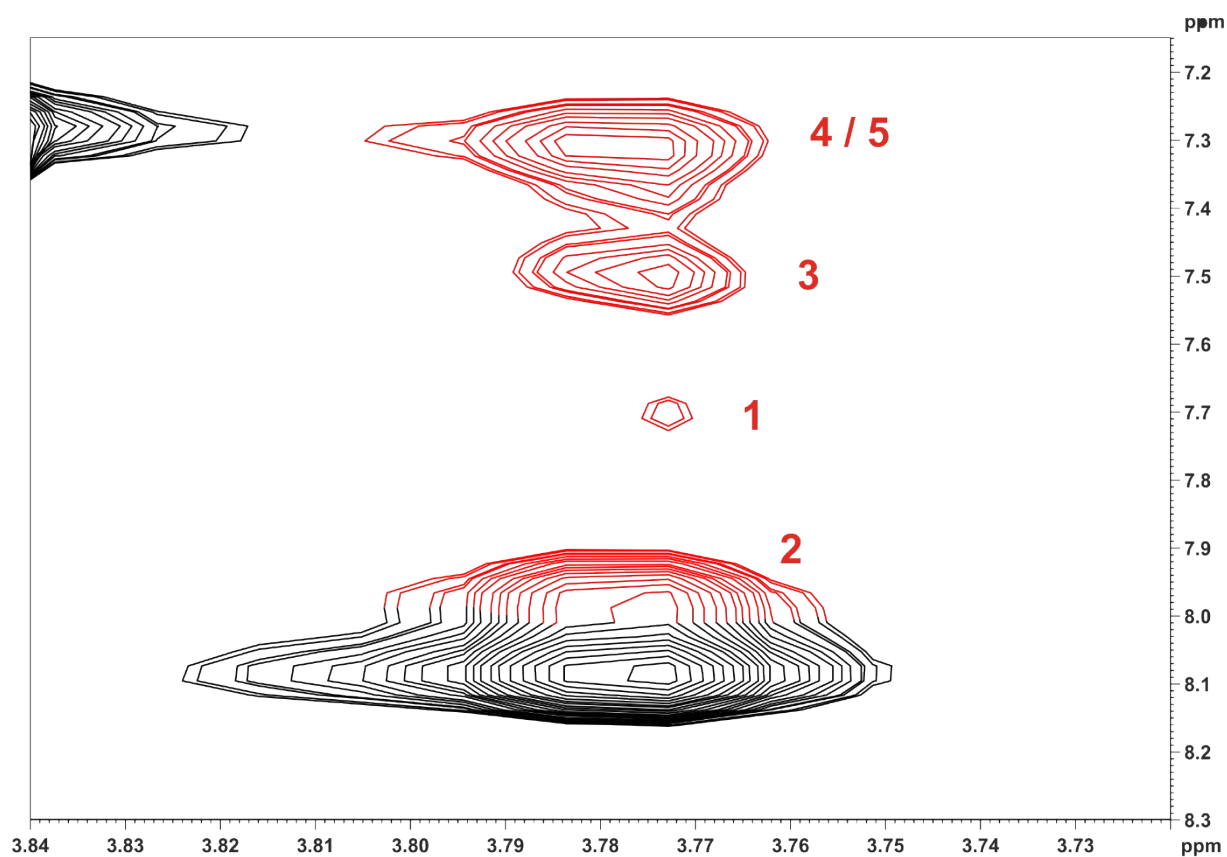
S34. Type I TRIM/5Z Complex



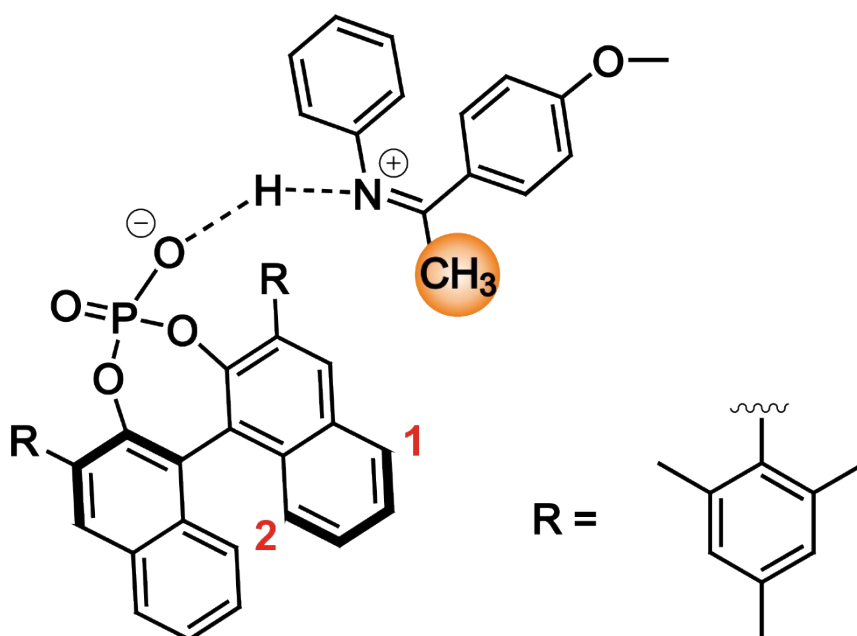
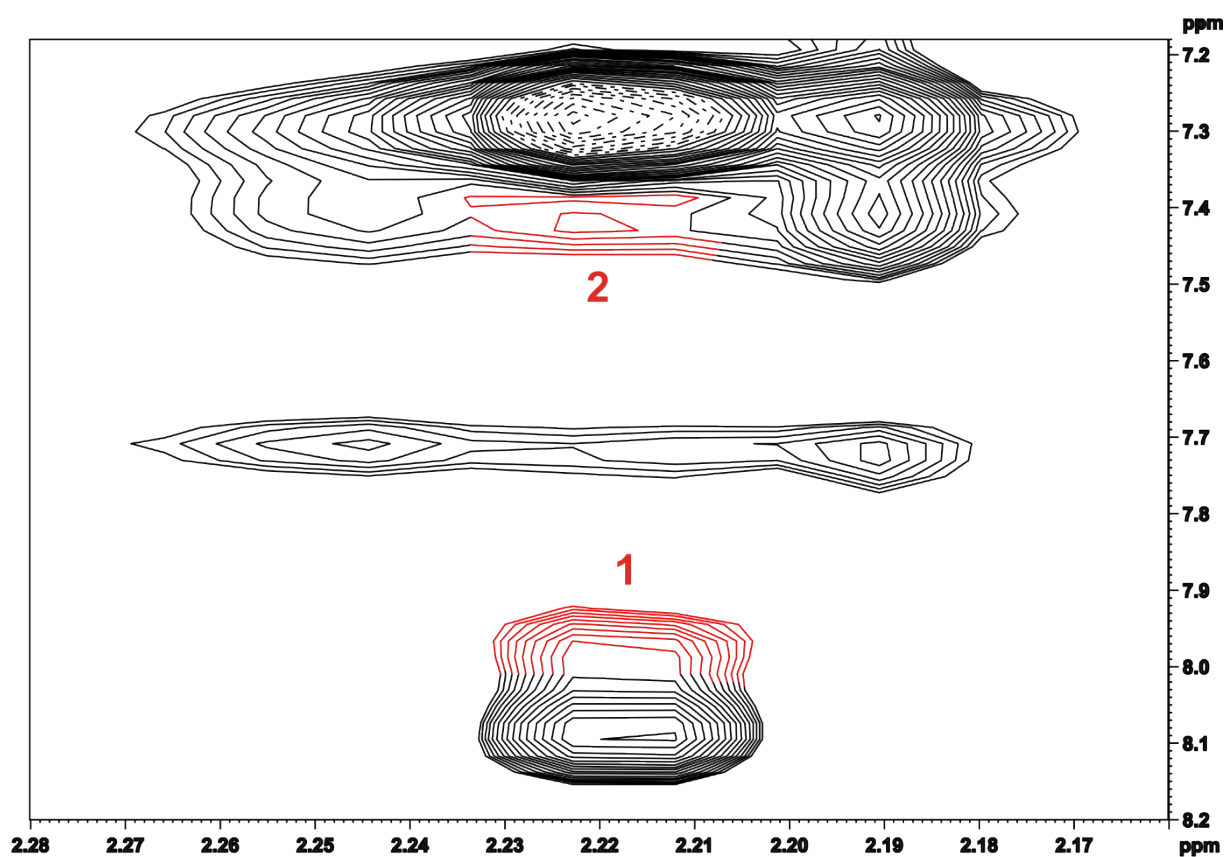
S35. Type II TRIM/5EZ Complexes



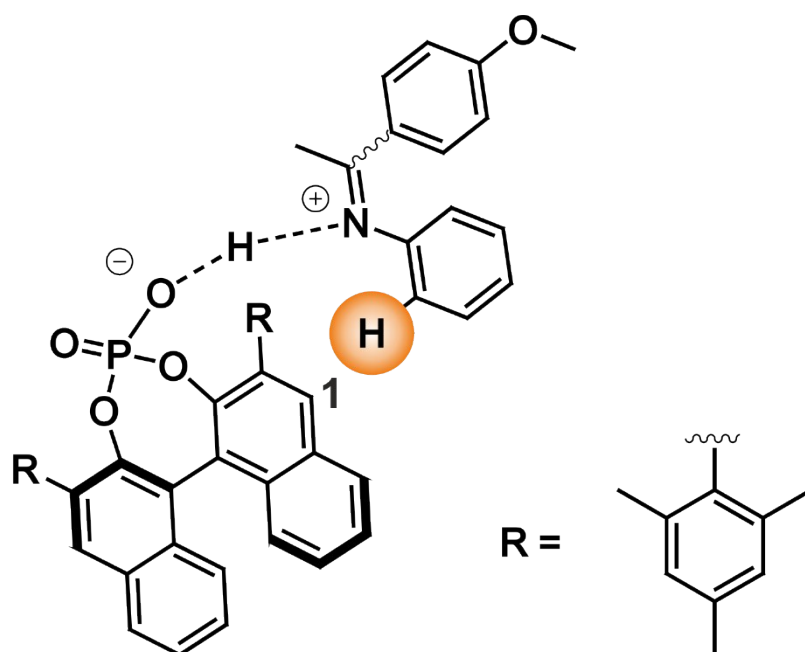
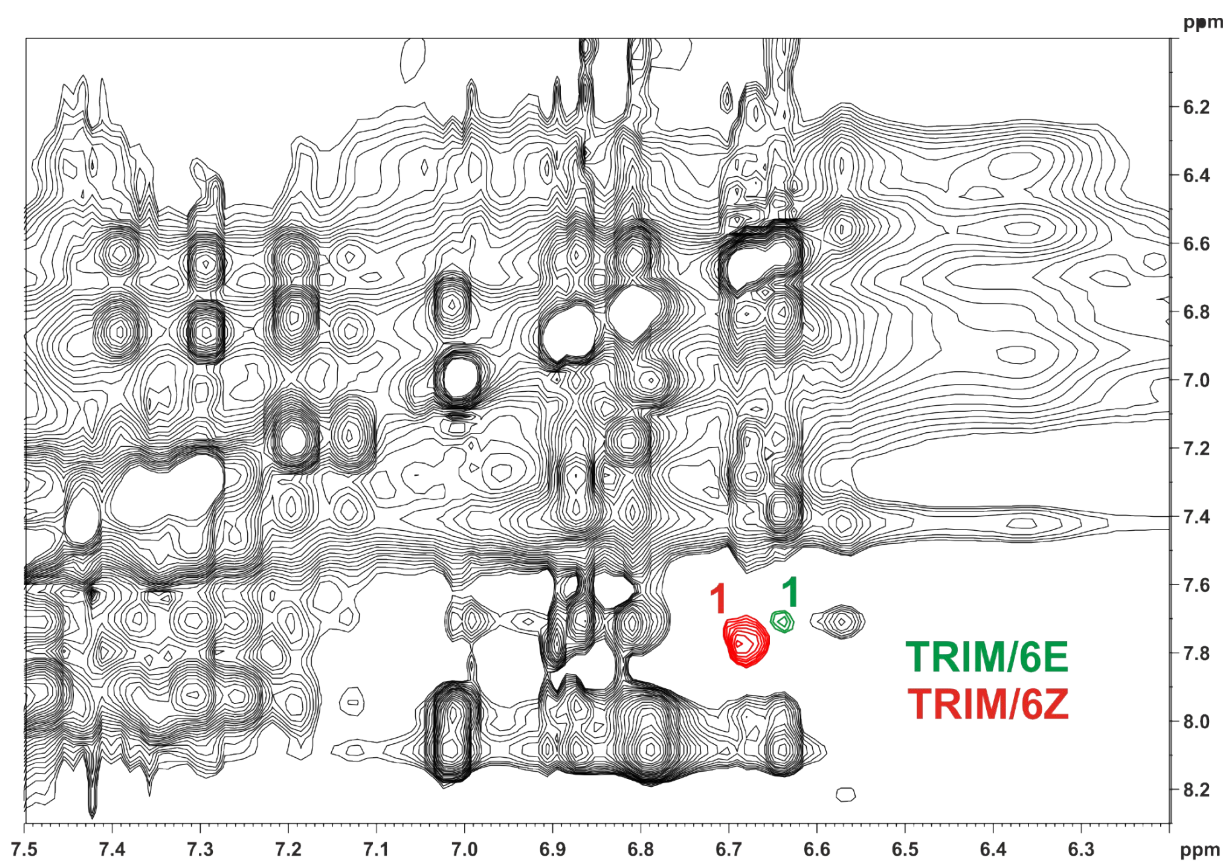
S36. Type I TRIM/6E Complexes



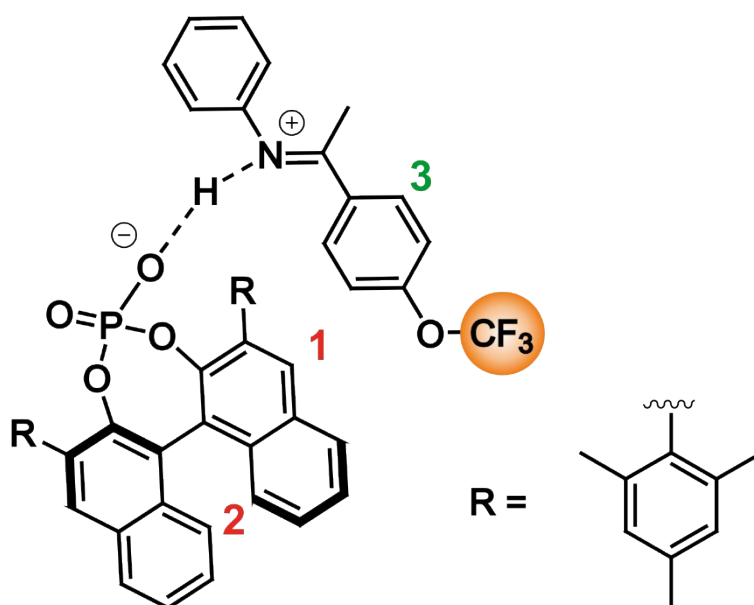
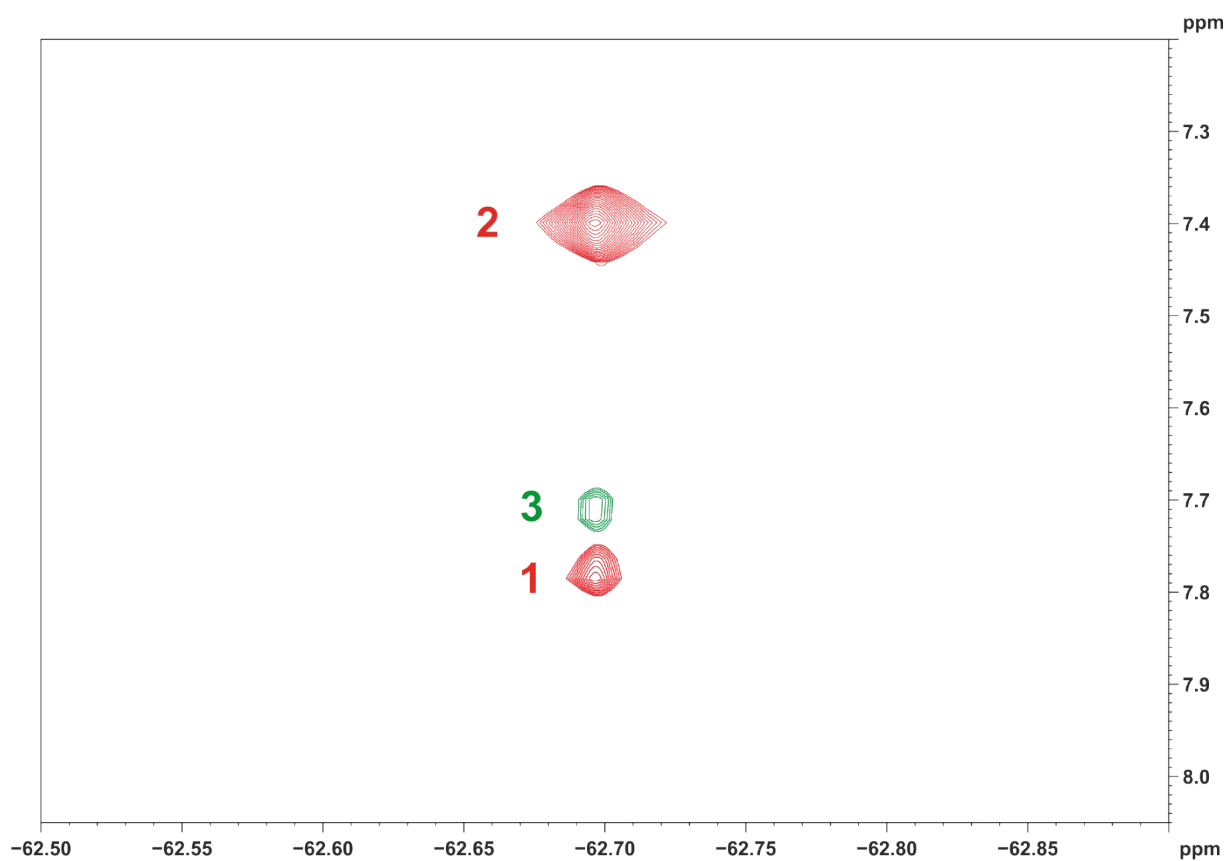
S37. Type I TRIM/6Z Complexes



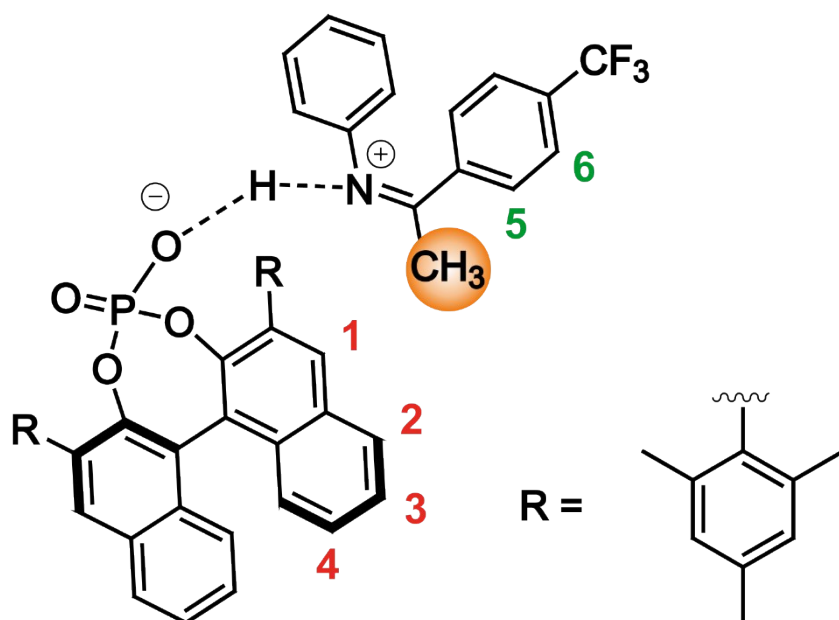
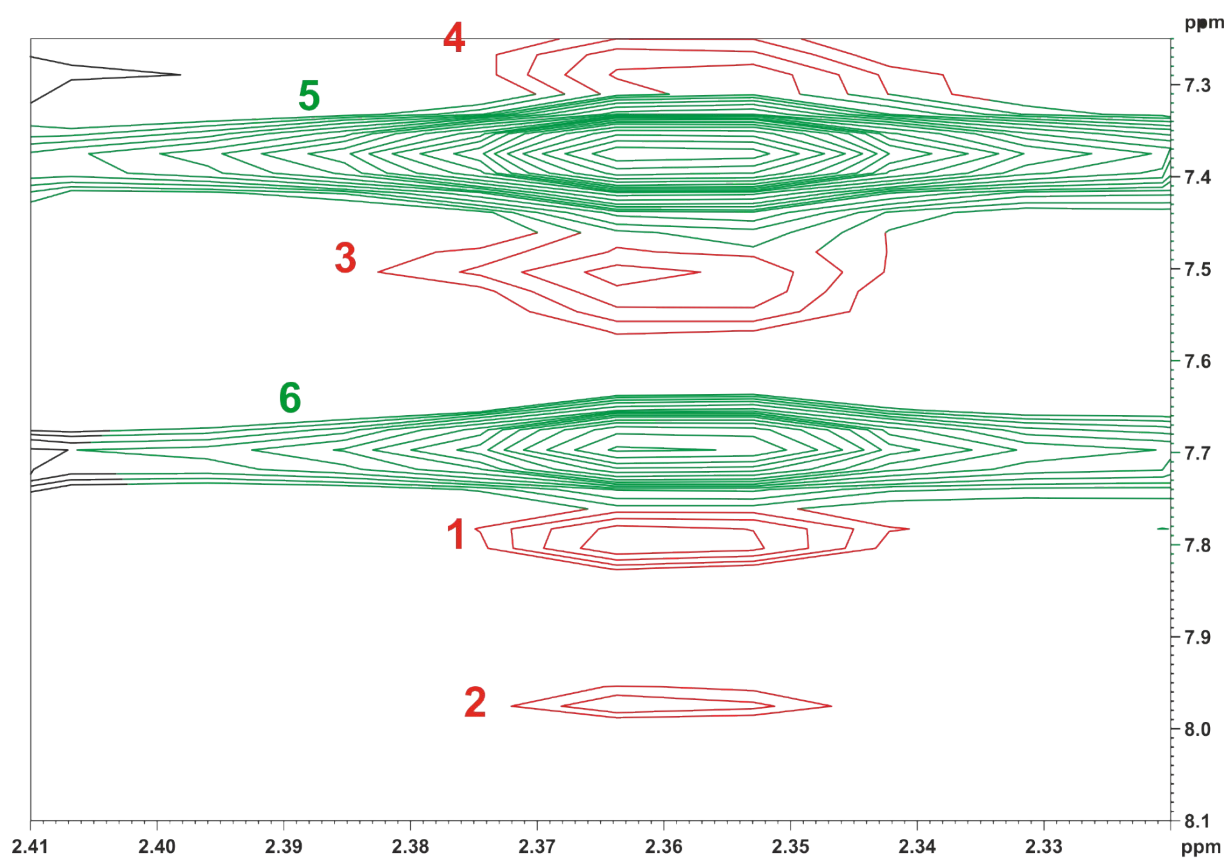
S38. Type II TRIM/6EZ Complexes



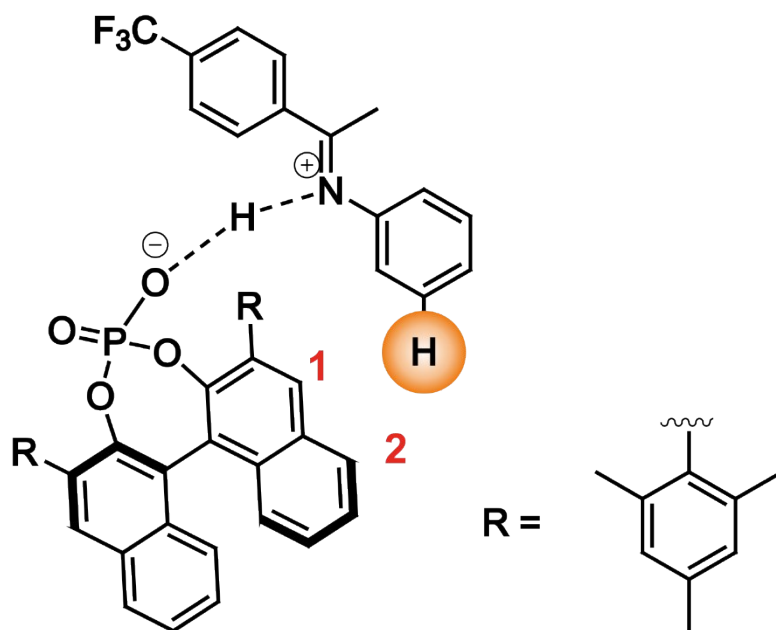
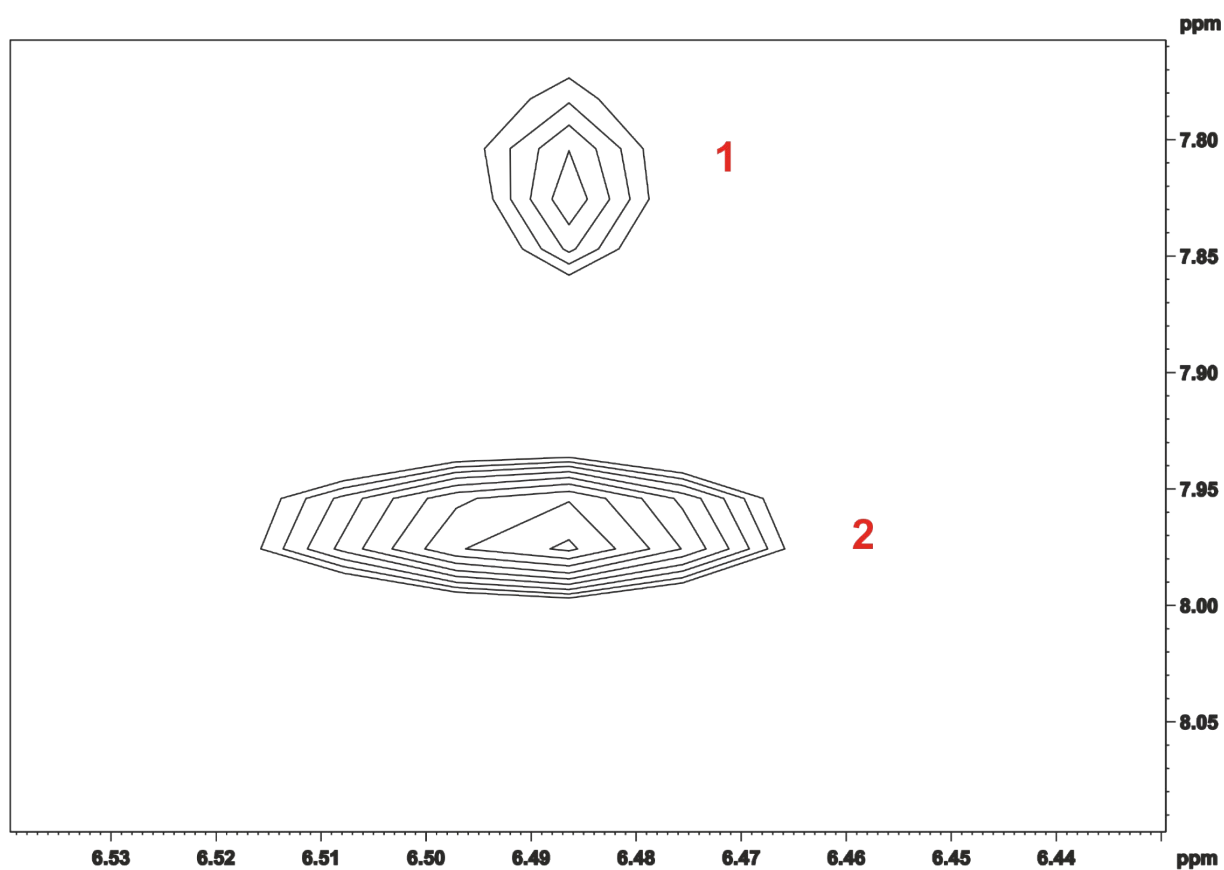
S39. Type I TRIM/7E Complex



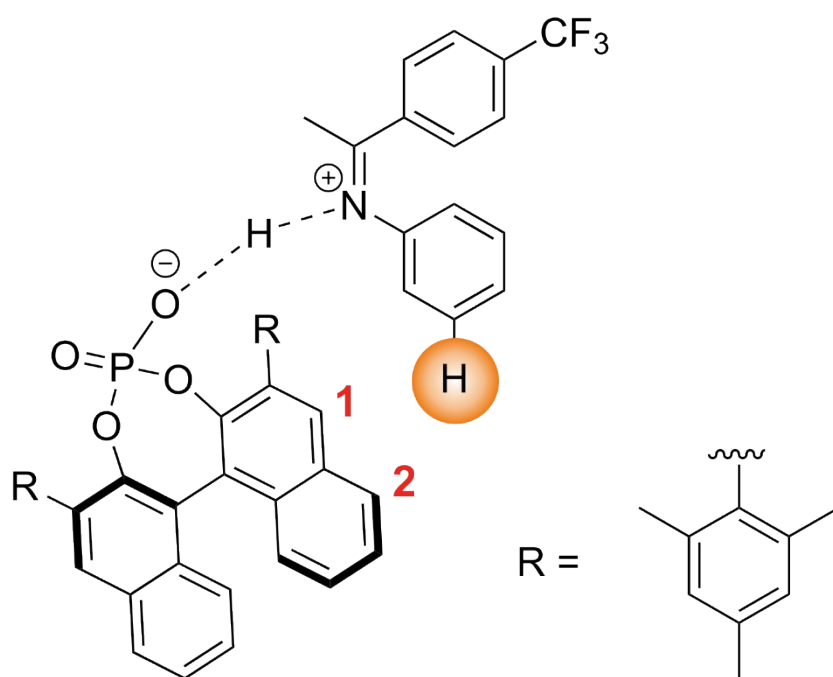
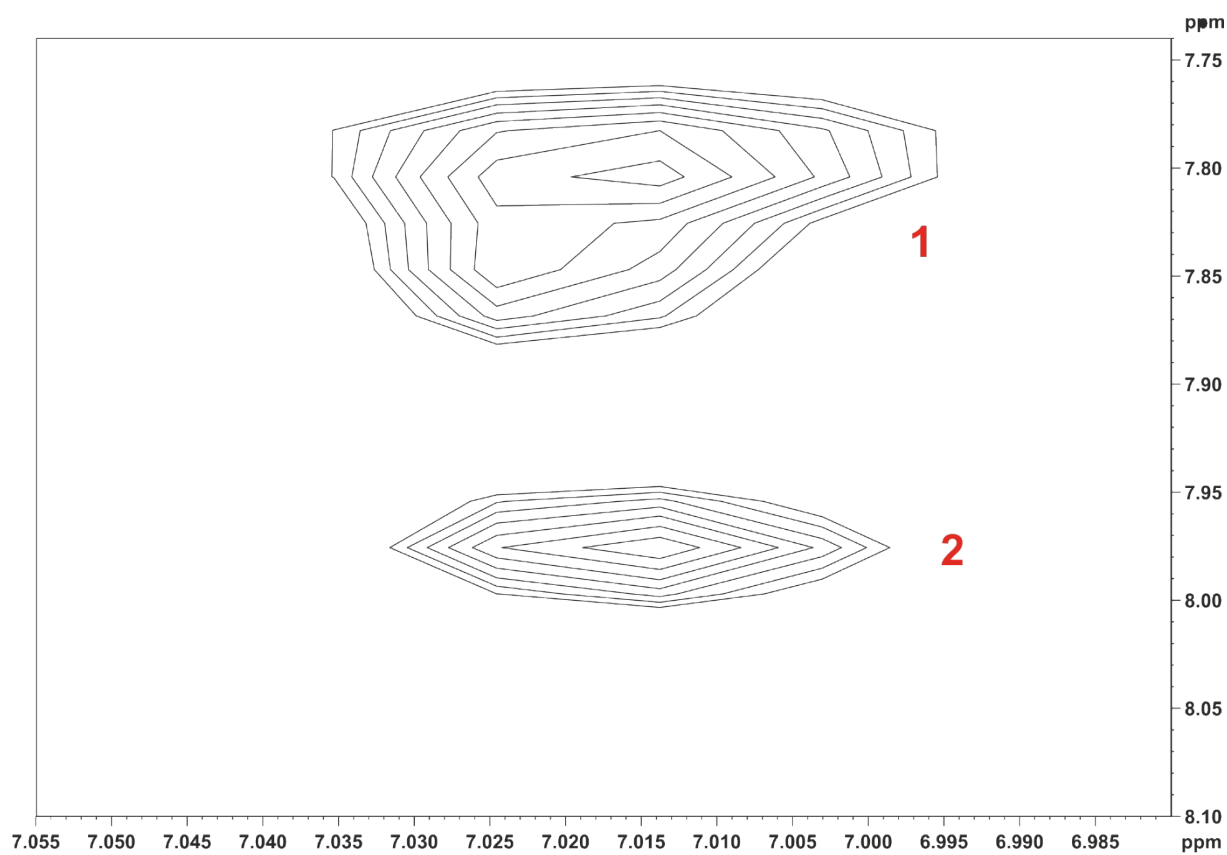
S40. Type I TRIM/7Z Complex



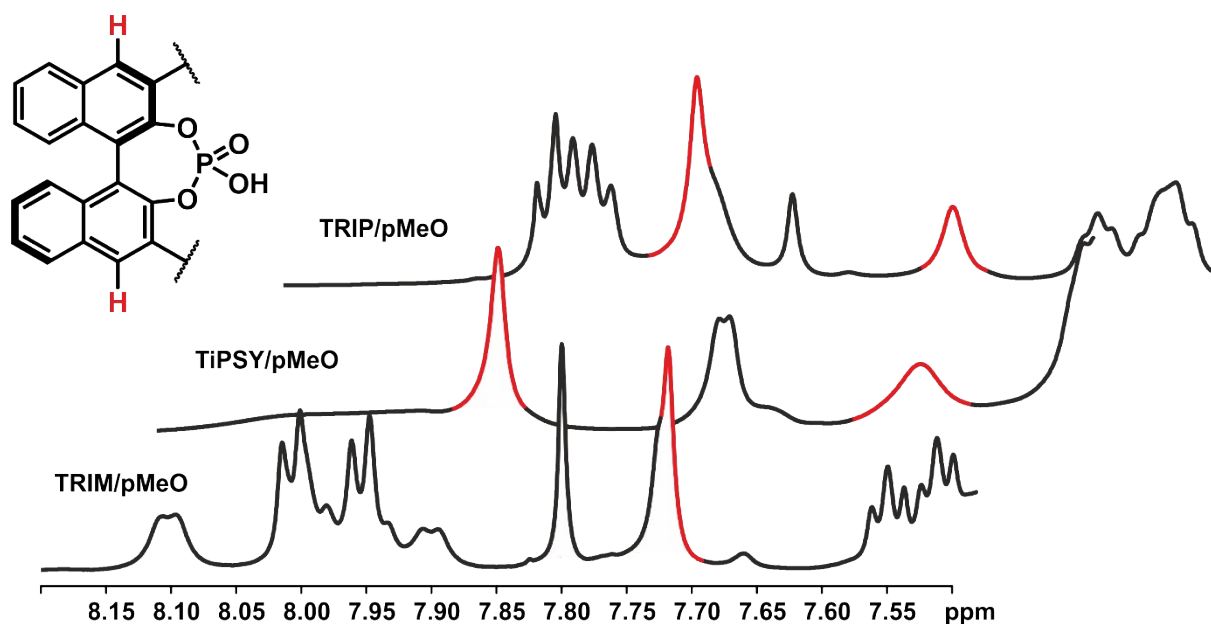
S41. Type II TRIM/7E Complex



S42. Type II TRIM/7Z Complex



S43 Exchange pathways in binary TRIM/imine complexes



1D ¹H spectra of catalysts TRIP, TiPSY and TRIM/6 at 180 K in CD₂Cl₂ at 600 MHz; for TRIP and TiPSY, a splitting of the signal sets of the BINOL backbone is seen, as exemplarily shown for one proton labelled in red; TRIM/imine complexes only show one averaged set of signals for both halves of the backbone.

A possible reason for this averaging in the TRIM/imine complexes might be a faster exchange between the free imine and the imine inside the complex or an additional exchange pathway between structures *Type I E* and *Type II E* via rotation of the imine similar to the Z-structures. The latter might be enabled due to the reduced Area(Θ) value of TRIM.^[9]

DOSY measurements for TRIM dimer

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 at 180 K.^[10] TMS was used to reference the viscosity of the solvent. 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 2.9 – 3.1 ms, 6.0 ms and 7.0 ms were found for TMS, TRIM/**7** and [TRIM/**7E**]₂, respectively. For each species, twenty spectra with linear varying gradient strength of 5% - 95% or 10% - 95% have been measured. Either the H-bond proton signals or the methyl-groups of the 3,3'-substituents have been used as probes. 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] The sigmoidal fit provided the translational self-diffusion coefficients D_i listed in Table S33. The molecular radii were derived by the Stokes-Einstein equation.^[12]

$$D_i = \frac{k_B T}{\pi \eta r_H}$$

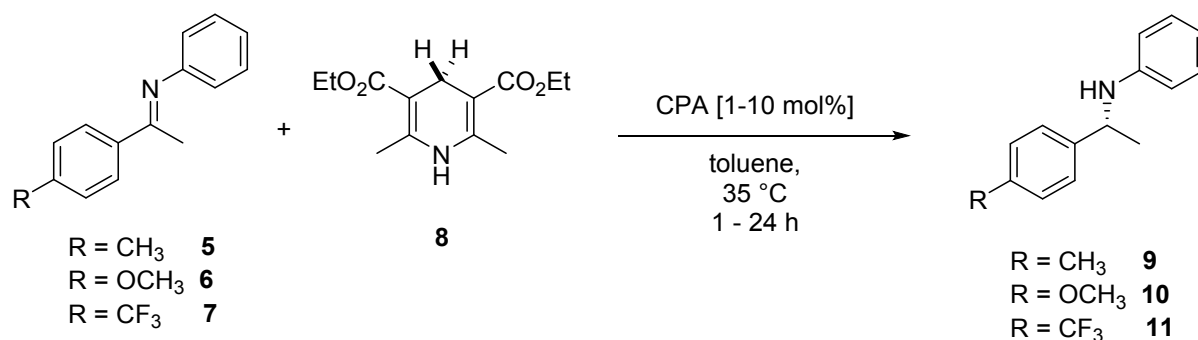
D_i is the self-diffusion coefficient derived by the measurement, η is the viscosity of the solvent and r_H is the hydrodynamic radius of the observed molecule. Due to the three-side exchange between [TRIM/**7E**]₂, TRIM/**7E** and free, not complexated TRIM and **7**, the absolute obtained self-diffusion coefficients are not meaningful. If two molecules A and B with different diffusion constants are in slow exchange with each other, the observed diffusion coefficients are a combination of the intrinsic diffusion coefficients of A and B without exchange, weighed with the respective lifetimes of A and B.^[13,14] Hence, only a qualitative interpretation of the DOSY spectra was possible. Molecular radii of 9.54 and 12.57 Å were found for TRIM/**7E** and [TRIM/**7E**]₂, respectively. The derived larger molecular size clearly corroborates the assignment as a dimer.

S44. Self-diffusion coefficients

Table S44: Measured self-diffusion coefficients and derived molecular radii. Entry 1-6: SW = 22 Hz, O1P = 2.00 ppm, gradient strength 5-95% linear; entry 7.11: SW = 22 Hz, O1P = 9.00 ppm, gradient strength 10-95% linear. No diffusion coefficients based on the H-Bond proton signals of [TRIM/7E]₂ could be derived due to low signal intensities. Diffusion coefficients of different signals of the same species were averaged.

Entry	Species	p16 [ms]	probe signal [ppm]	D _i [m ² /s] · 10 ⁻¹²	Averaged	r _H [Å]
1	TMS	3.10	0.00	16.81		
2	TRIM/7EZ	6.00	2.22	3.645		
3	TRIM/7EZ	6.00	2.12	3.732	3.693	9.54
4	TRIM/7EZ	6.00	2.00	3.702		
5	[TRIM/7E] ₂	7.00	1.62	2.774	2.761	12.57
6	[TRIM/7E] ₂	7.00	1.02	2.748		
7	TMS	3.00	0.00	19.35		
8	TRIM/7Z	6.00	17.83	4.334	4.393	9.25
9	TRIM/7Z	6.00	17.70	4.419		
10	TRIM/7E	6.00	17.58	4.361		
11	TRIM/7E	6.00	17.45	4.457		

S45 Determination of ee values



A Schlenk tube was dried at 350 °C under reduced pressure for several minutes. Imine **5-7** (0.1 mmol, 1.0 eq.), the CPA catalyst (0.01 eq. or 0.1 eq. for TiPSY) and Hantzsch Ester **8** (36.5 mg, 0.14 mmol, 1.4 eq.) were weighed into the tube. The tube was evacuated and flushed with Argon three times. Under Argon flow, anhydrous toluene (1.0 mL) was added. The reaction was stirred at 35 °C for 1 – 24 h. 0.1 – 0.2 mL of the crude reaction mixture was taken and quenched by addition to a vial filled with hexane (2.0 mL) and NEt_3 (10 μL , 7.3 μg , 0.072 mmol, 7.2 – 72 eq. based on the catalyst). The mixture was filtered and analysed by chiral HPLC (see S47 for further details).

Table S45: ee values of the transfer hydrogenation of imines 5-7 with Hantzsch Ester catalysed by various CPAs.

Catalyst	Imine 5		
	major [Area%]	minor [Area%]	ee [%]
TRIP	92.2	7.8	84
TRIFP	87.2	12.7	75
TiPSY	95.1	4.9	90
1-naph	79.4	20.6	59
9-phen	78.0	21.9	56
TRIM	85.6	14.3	71
Catalyst	Imine 6		
	major [Area%]	minor [Area%]	ee [%]
TRIP	93.0	7.0	86
TRIFP	87.0	13.0	74
TiPSY	95.5	4.5	92
1-naph	78.1	21.9	56
9-phen	77.8	22.2	56
TRIM	85.0	15.0	70
Catalyst	Imine 7		
	major [Area%]	minor [Area%]	ee [%]
TRIP	91.7	8.3	83
TRIFP	95.6	4.3	91
TiPSY	97.7	2.3	95
1-naph	73.4	26.6	47
9-phen	73.0	27.0	46
TRIM	78.2	21.8	56

S46 Correlation of ee with CPA parameters

Table S46: List of experimental ee values, E- and Z-imine populations in the binary CPA/imine complexes and steric descriptors as used by Goodman.^[15]

Catalyst	Imine									Steric Descriptors	
	5			6			7			AREA(Θ)	Rot. Barrier
	ee	% E	% Z	ee	% E	% Z	ee	% E	% Z	[°]	[kcal/mol]
TRIP	84	67	33	86	77	23	83	86	14	51	28.4
TRIFP	75	70	30	74	81	19	91	69	31	62	2.02
TIPSY	90	56	44	92	70	30	95	71	29	29	1.13
TRIM	71	47	53	70	49	51	56	55	45	61	21.58
1-naph	56	-	-	56	-	-	46	-	-	62	13.63
Phen	59	-	-	56	-	-	47	-	-	48	14.45

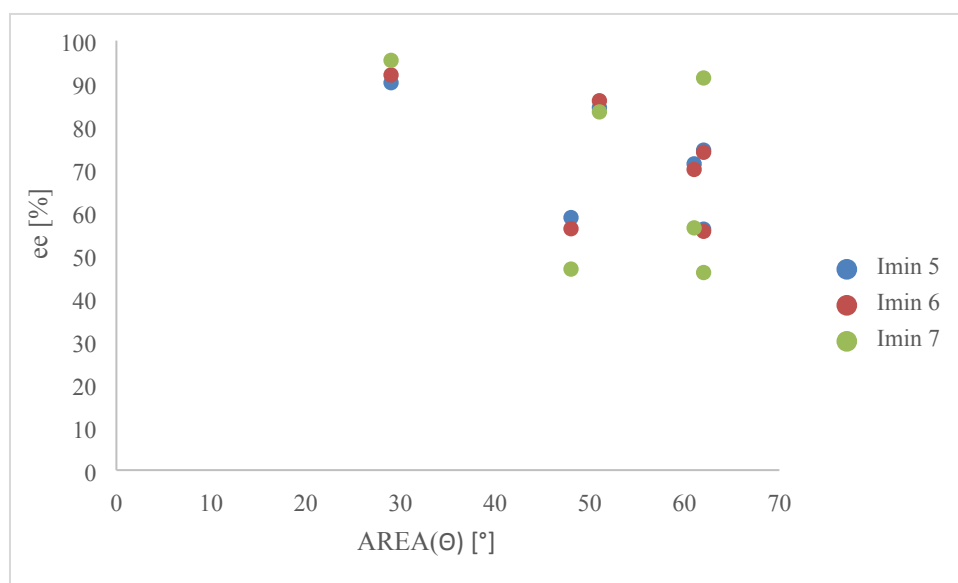


Figure S46.1: Plot of the ee values of the transfer hydrogenation of imines **5-7** catalyzed by TRIP, TRIFP, TIPSY, TRIM, 1-naph and 9-phen against the AREA(Θ) value computed by Goodman.^[15] No correlation is observed.

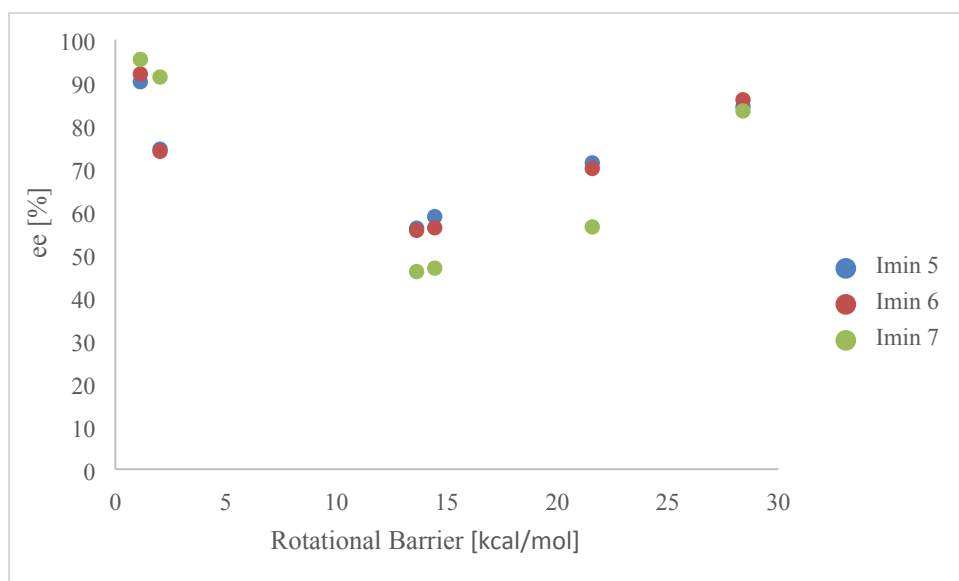


Figure S46.2: Plot of the ee values of the transfer hydrogenation of imines 5-7 catalyzed by TRIP, TRIFP, TiPSY, TRIM, 1-naph and 9-phen against the Rotational Barrier value computed by Goodman.^[15] No linear correlation is observed.

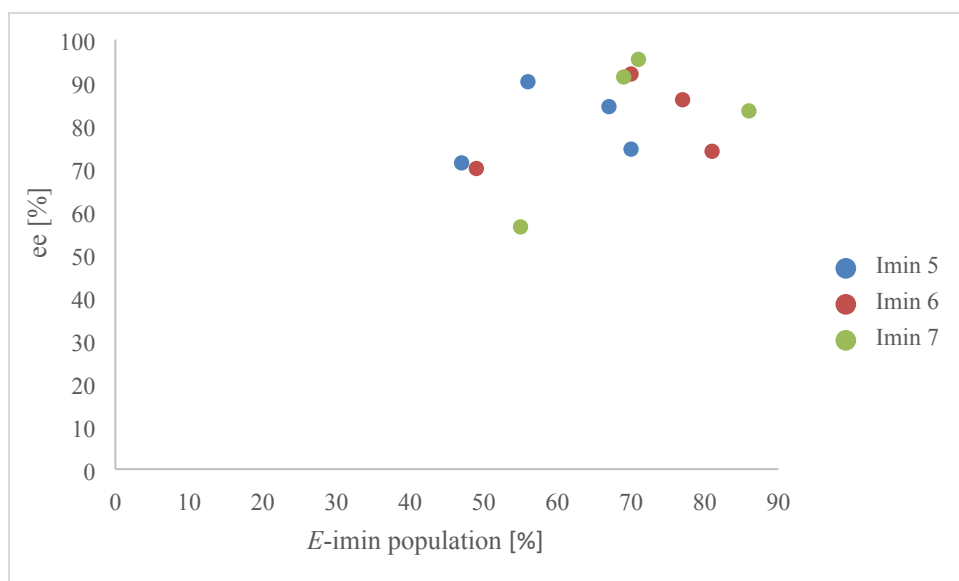


Figure S46.3: Plot of the ee values of the transfer hydrogenation of imines 5-7 catalyzed by TRIP, TRIFP, TiPSY, TRIM, 1-naph and 9-phen against the experimentally observed population of the *E*-imine in the binary complex. No correlation is observed.

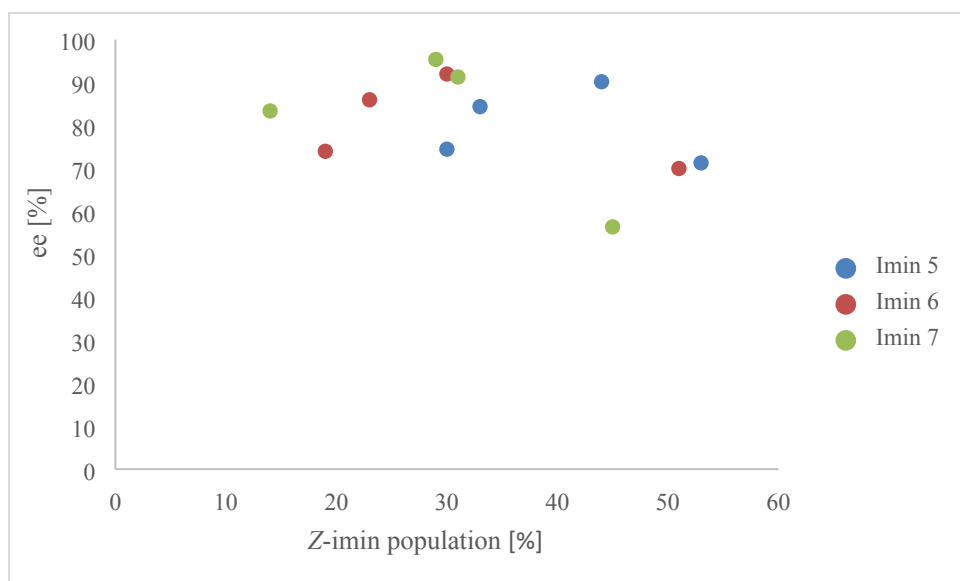


Figure S46.4: Plot of the ee values of the transfer hydrogenation of imines 5-7 catalyzed by TRIP, TRIFP, TiPSY, TRIM, 1-naph and 9-phen against the experimentally observed population of the Z-imine in the binary complex. No correlation is observed.

S47 HPLC analysis

To determine the ee values of imines **5-7**, identical HPLC equipment and conditions have been used as previously employed by our group.^[16] For further details, especially preparation and separation of the racemic amines **9-11** see the supporting information of the cited literature.

Enantiomeric excess values (ee) of products were determined by HPLC on chiral stationary phase employing an Agilent 1290 Infinity LC system equipped with a binary pump, autosampler and a photodiode array detector and using CHIRALCEL OD-H and CHIRALPAK IA and IC columns.

Amine 9: The ee was determined by CSP-HPLC, CHIRALCEL OD-H column, eluent *n*-hexane/*i*-propanol 98/2, flow 0.6 mL/min, retention times: τ_1 = 13.34 min, τ_2 = 14.40 min, column compartment temperature 20 °C, λ = 220 nm.

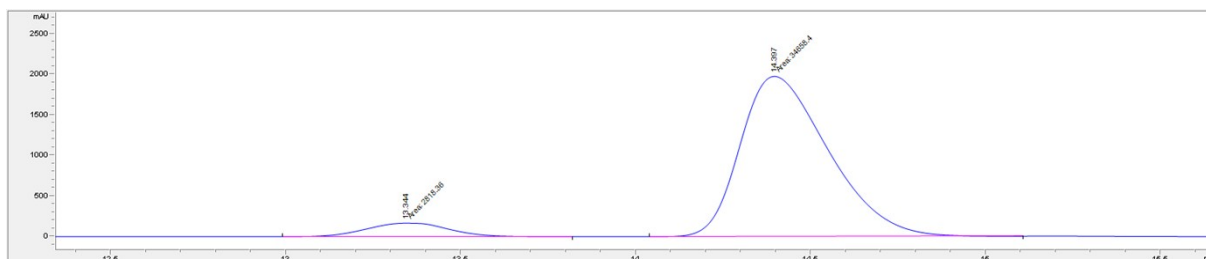
Amine 10: The ee was determined by CSP-HPLC, CHIRAPACK IC column, eluent *n*-hexane/*i*-propanol 99/1, flow 0.9 mL/min, retention times: τ_1 = 8.22 min, τ_2 = 8.59 min, column compartment temperature 20 °C, λ = 220 nm.

Amine 11: The ee was determined by CSP-HPLC, CHIRALPACK IA column, eluent *n*-hexane/*i*-propanol 98/2, flow 0.9 mL/min, retention times: τ_1 = 12.84 min, τ_2 = 13.89 min, column compartment temperature 20 °C, λ = 220 nm

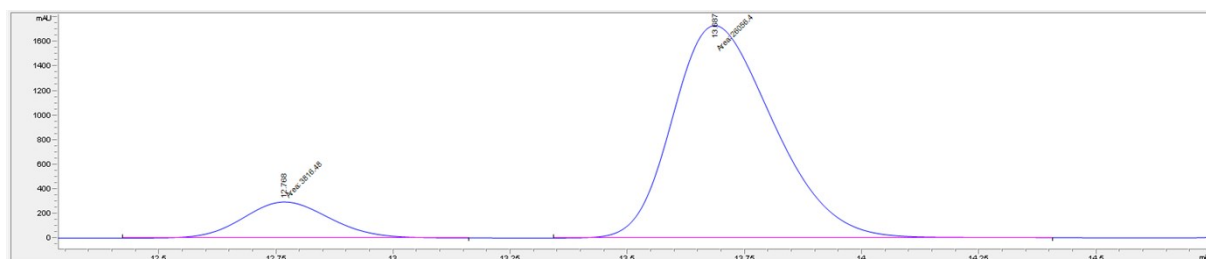
Chromatograms:

Amine **9**, catalyzed by

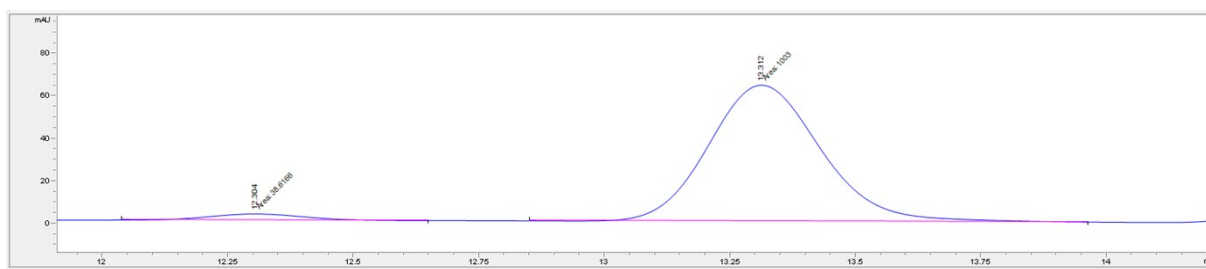
TRIP



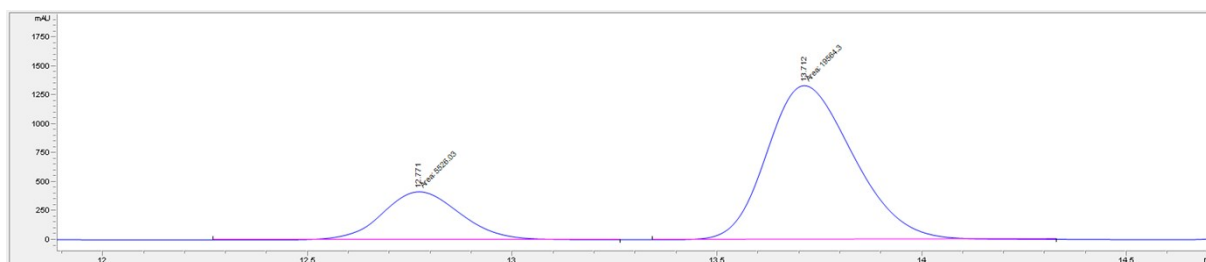
TRIFP



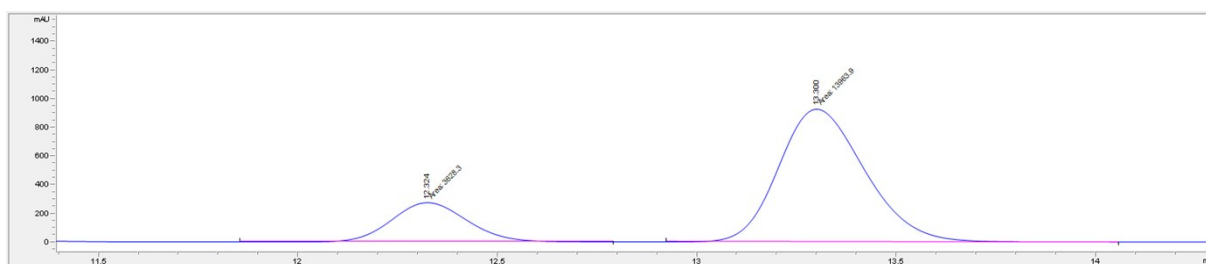
TiPSY



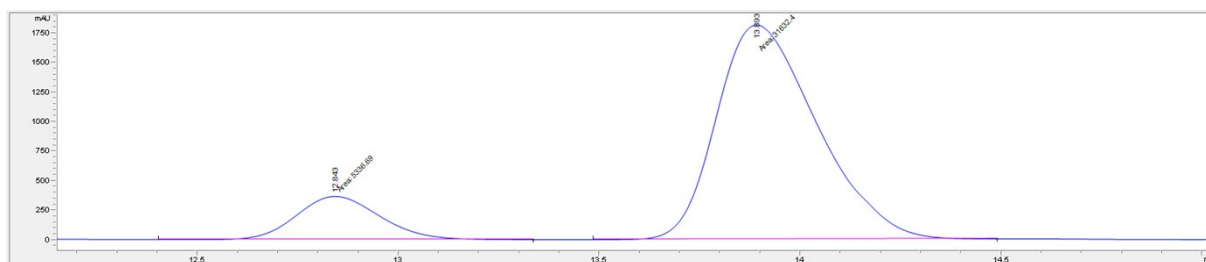
1-naph



9-phen

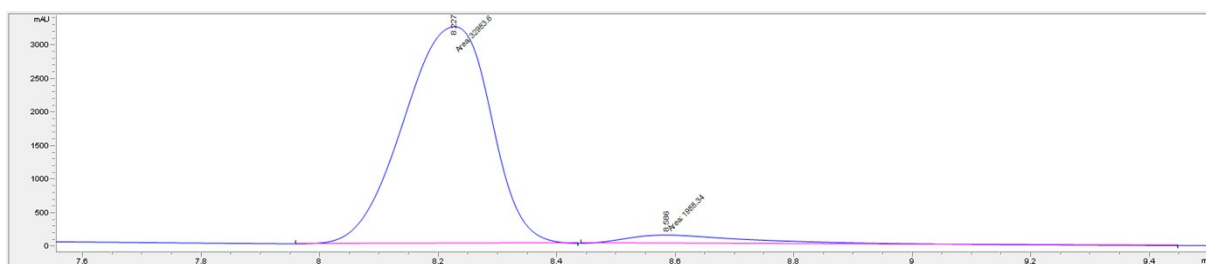


TRIM

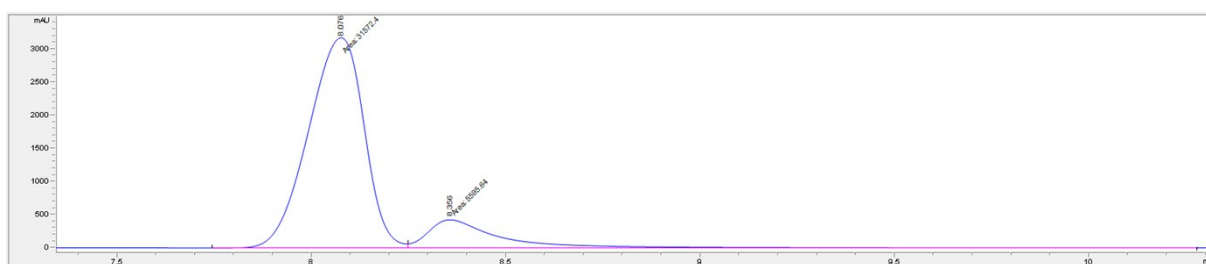


Amine **10**, catalyzed by

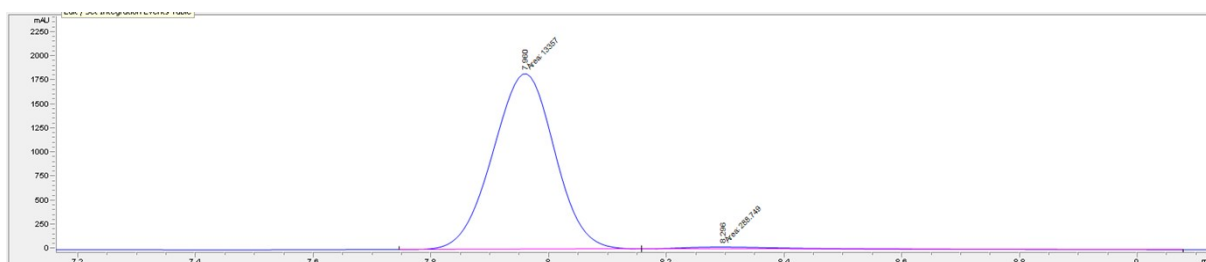
TRIP



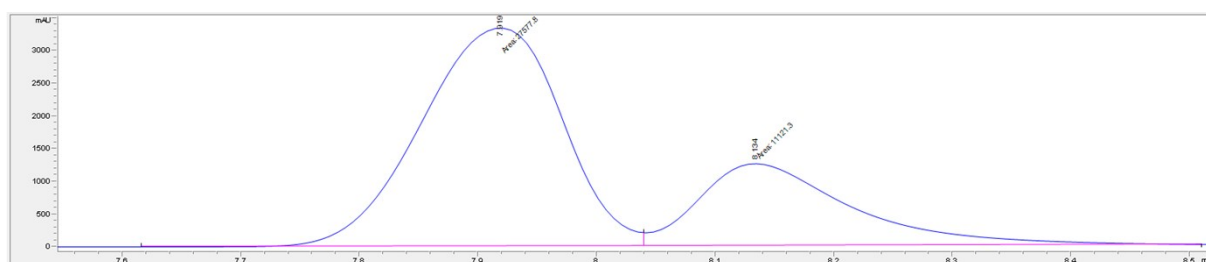
TRIFP



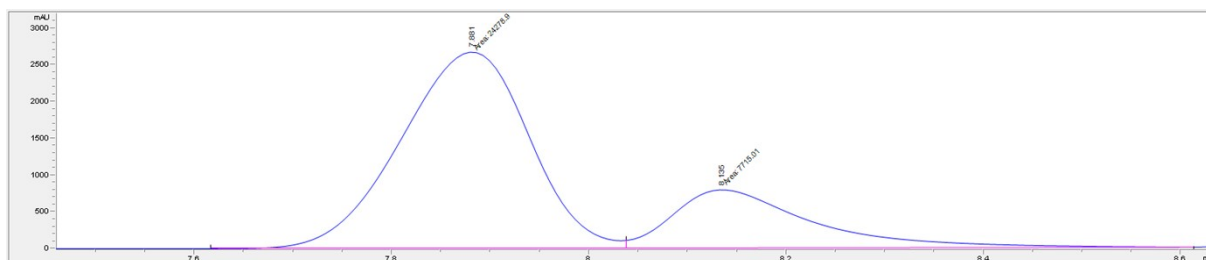
TiPSY



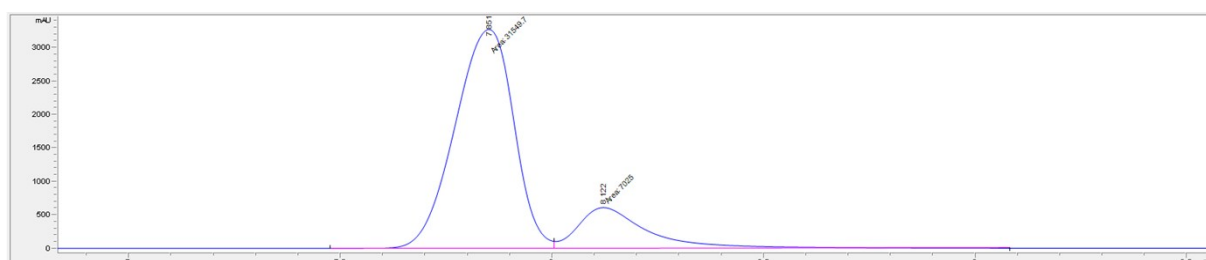
1-naph



9-phen

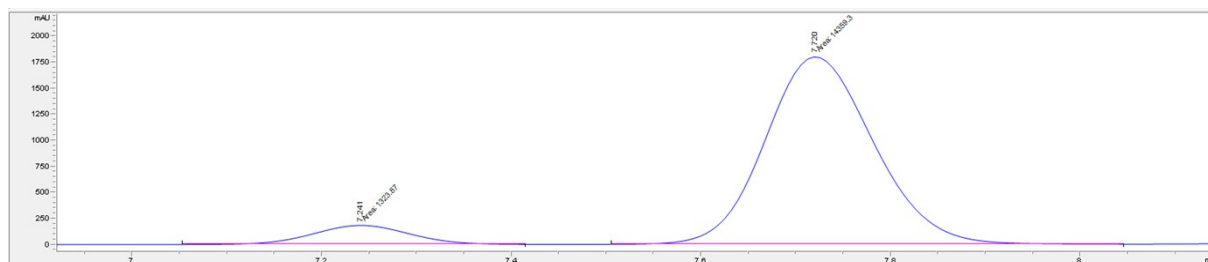


TRIM

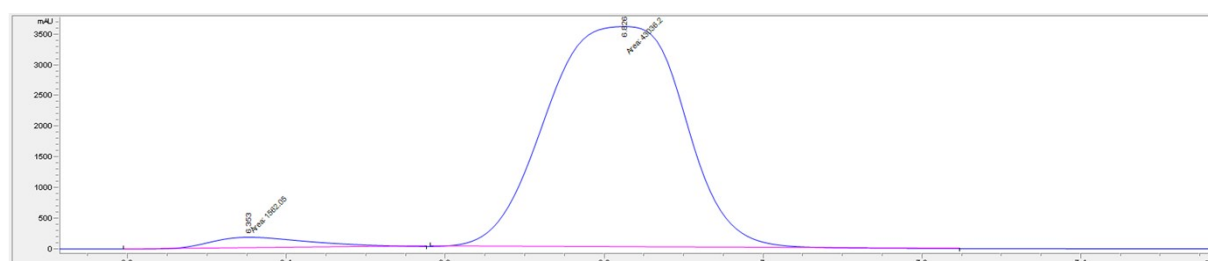


Amine **11**, catalyzed by

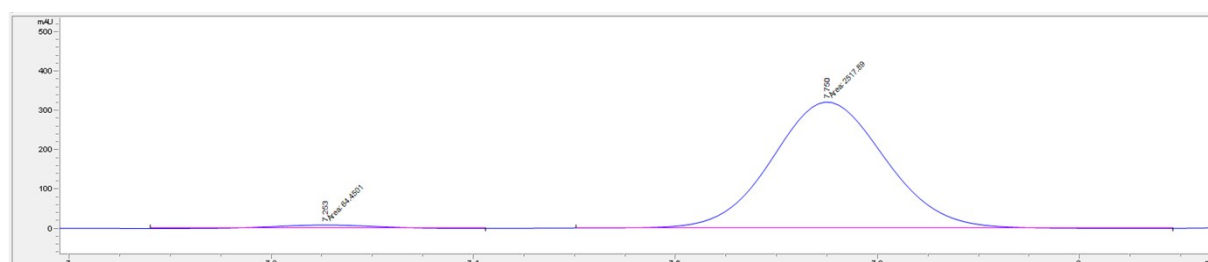
TRIP



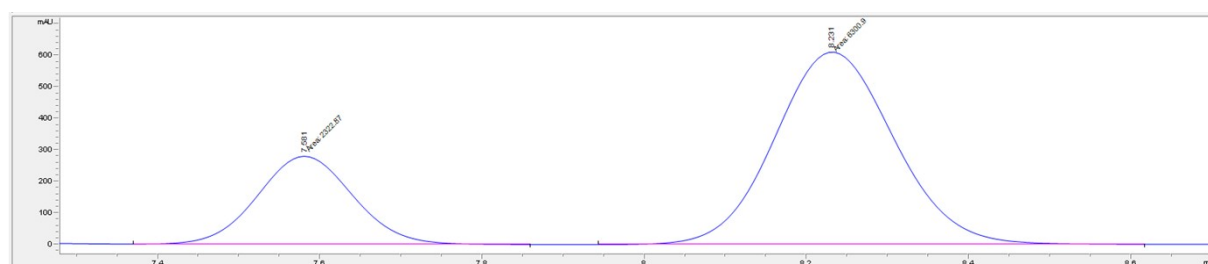
TRIFP



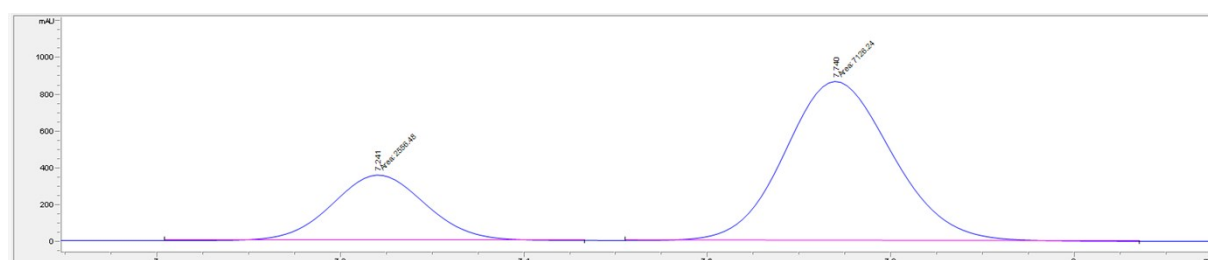
TiPSY



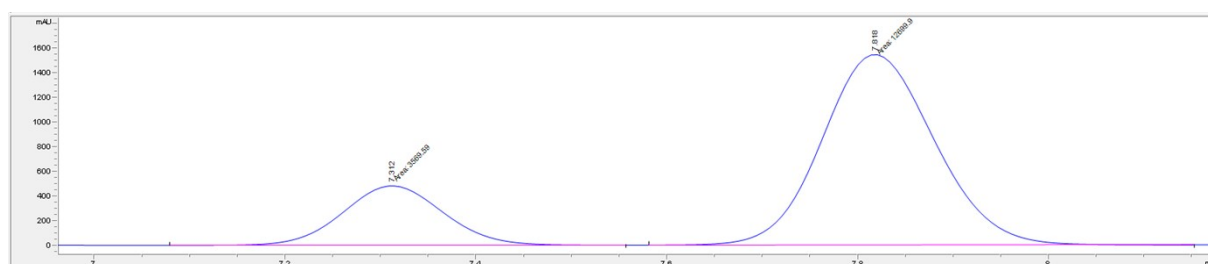
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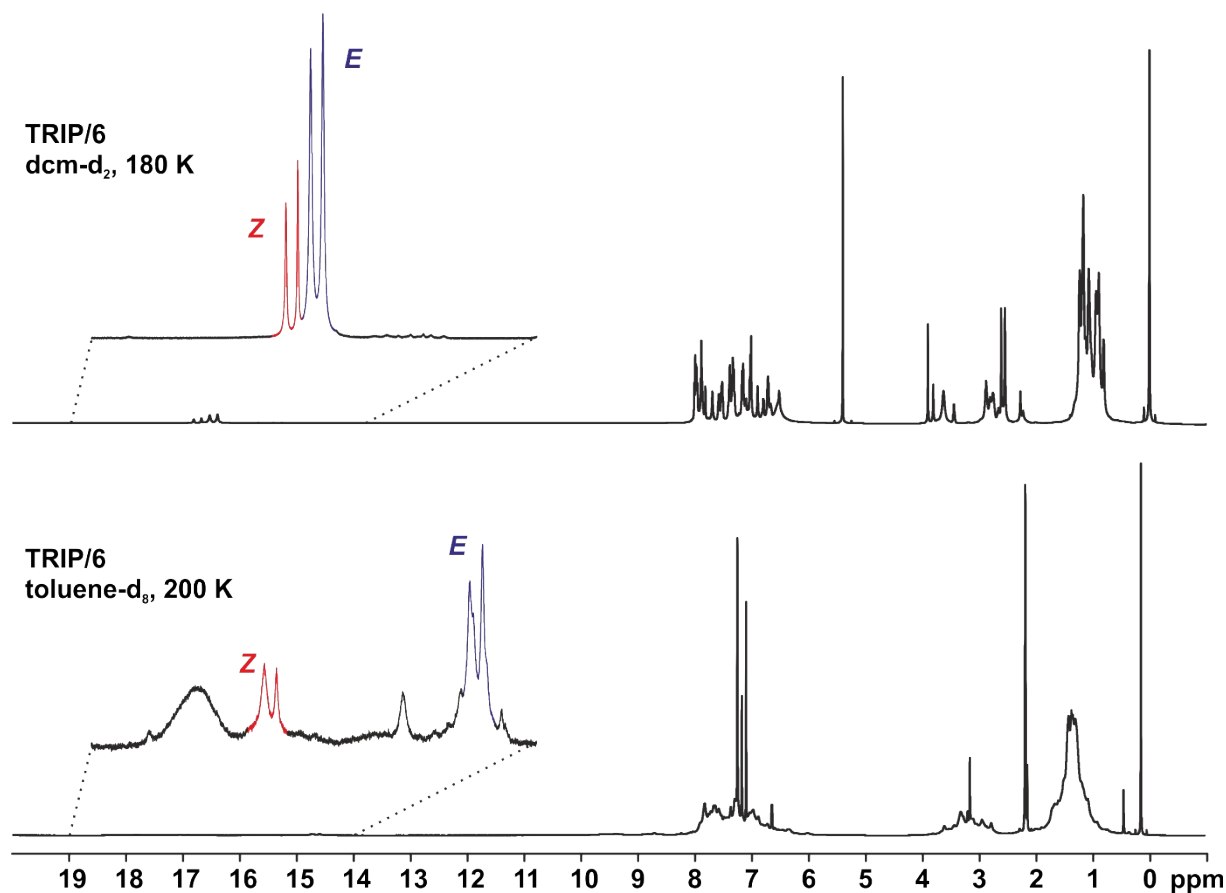
9-phen



TRIM



S48 Effects of different solvents on *E/Z* ratios



When using toluene-d₈ as solvent, the line widths of all catalyst and imine signals increase significantly, compared to dichloromethane-d₂. In addition, the *E/Z* ratio changes from 77:23 (dcm) to around 70:30 (toluene), illustrating the strong influence of the solvent on this ratio. No trend can be observed for *E/Z* ratios in different solvents

Table. *E/Z* ratios of investigated complexes in different solvents at 180-200 K.

Complex	CD ₂ Cl ₂	Toluene-d ₈	Freonic mixture
TRIP/5	77:23	71:29	78:22
TRIP/6	67:33	n.d.	77:23
TRIFP/6	81:19	n.d.	80:20

S49 Computational details

Binary complexes consist of TiPSY, TRIP and TRIFP with imines **5**, **6**, **7** were optimized at TPSS-D3/def2-SVP level of theory in continuum of CH₂Cl₂.^[17,18] The dielectric constant of the solvents was modified to 16.20 to mimic low temperature NMR measurement. Subsequently all minima were verified by frequency analysis (zero imaginary vibrational mode) and thermochemical corrections were added. Single point calculations at SCS-MP2/CBS level of theory (for extrapolation procedure see SI) were employed on top of the optimized geometry.^[19] Software used for the optimization was Gaussian09 D.01.^[20] For single points, ORCA 3.0.3 was used.^[21] For the basis set extrapolation procedure Eq.1-3 were used with the basis set def2-SVP and def2-TZVP (X=2,3). $\alpha=10.39$, $\beta=2.40$.

$$E_{\text{SCF}}^X = E_{\text{SCF}}^{\infty} + Ae^{-\alpha\sqrt{X}} \quad \text{Eq. 1}$$

$$E_{\text{corr,MP2}}^{\infty} = \frac{X^{\beta} E_{\text{corr,MP2}}^X - (X-1)^{\beta} E_{\text{corr,MP2}}^{X-1}}{X^{\beta} - (X-1)^{\beta}} \quad \text{Eq. 2}$$

$$E_{\text{MP2}}^{\infty} = E_{\text{SCF}}^{\infty} + E_{\text{corr,MP2}}^{\infty} \quad \text{Eq. 3}$$

Table S1. Boltzmann averaged G₁₈₀ SCS-MP2/CBS of the binary complexes

S50. Optimized Geometry (most stable conformation)

TRIP/5 Type I E

```
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TRIP/5 Type II E

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TRIP/5 Type I Z

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TRIP/5 Type II Z

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TRIP/6 Type I E

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TRIP/6 Type II E

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TRIP/6 Type I Z

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TRIP/6 Type II Z

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TRIP/7 Type II E

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TRIP/7 Type II Z

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TiPSY/5 Type I E

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(C71H56N1O4P1Si2)]\@

TiPSY/5 Type II E

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TiPSY/5 Type I Z

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TiPSY/5 Type II Z

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\\@

TiPSY/6 Type I E

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 14,-1.4415810911,4.0208643768\H,-2.6786631083,0.1321329405,3.092697844
 1\C,-4.9121277102,-2.3237483933,3.9013029481\H,-6.5731684295,-2.965646
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TiPSY/6 Type II E

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TiPSY/6 Type I Z

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6,2.5704692831,-1.2605975884\C,3.2319978508,3.8851875525,0.2958061796\H,2.7211522711,1.9252866239,1.0480341741\C,5.0127290852,3.9641361691,-1.351292938\H,5.9237155687,2.0770196214,-1.8664789645\C,4.0475269685,4.6253478145,-0.5746079428\H,2.4825791532,4.3956463149,0.9113674572\H,5.6597857164,4.5351535526,-2.0270264893\H,3.9346262007,5.7132047404,-0.6444570768\C,4.4338602711,-0.8971230719,-2.0045363016\C,4.165139849,-0.152843526,-3.1743747913\C,4.5728555902,-2.300081541,-2.1338759097\C,4.0526549644,-0.7804362093,-4.425985328\H,4.0155999085,0.9301697561,-3.1112188773\C,4.4659138827,-2.930831056,-3.3808465013\H,4.7385419347,-2.9192808602,-1.2442663862\C,4.2061327854,-2.1704186614,-4.5332146988\H,3.8342675819,-0.18106258,-5.3172943495\H,4.5716664716,-4.0194563745,-3.4526971811\H,4.1141133193,-2.6625290767,-5.5081735143\C,-3.0525588927,-0.31655516,-2.4267717391\C,-2.2622506147,-0.8354777266,-3.4764020586\C,-3.5670421407,0.9942413682,-2.5679495821\C,-2.0031295148,-0.0786833596,-4.629966978\H,-1.815171496,-1.8294718073,-3.3852026931\C,-3.3133406808,1.7522550998,-3.7211129737\H,-4.1749310729,1.4336075178,-1.7687537006\C,-2.5328960838,1.2141344568,-4.7577859283\H,-1.3726248206,-0.4971859172,-5.4222387381\H,-3.7152631502,2.7682512657,-3.8057951347\H,-2.3280940387,1.8070987261,-5.6564593835\C,-4.1557219549,-0.3407385905,0.4921577944\C,-3.4226629053,-0.1895465785,1.6906418746\C,-5.4158860444,0.3007758765,0.4046053544\C,-3.918052136,0.5795915852,2.7559858251\H,-2.4510634426,-0.6842245351,1.8010556134\C,-5.9139458253,1.0731441122,1.4643233087\H,-6.0235658626,0.1878193764,-0.5015428864\C,-5.1637439979,1.2156069083,2.6430250575\H,-3.3281858115,0.6844604699,3.6733680048\H,-6.8883646661,1.566001778,1.371632151\H,-5.5497239391,1.8237198329,3.4684239964\C,-4.9688995099,-2.5158933494,-1.4977179582\C,-5.9045946904,-3.000919614,-0.5519084657\C,-5.1319690523,-2.9094026065,-2.8460264864\C,-6.9551776776,-3.8491775893,-0.9354268019\H,-5.8149110946,-2.7082800946,0.5014857778\C,-6.1815134106,-3.7569115628,-3.2351312087\H,-4.4340802976,-2.5450954882,-3.6092710791\C,-7.0950780598,-4.2299826078,-2.2797680036\H,-7.6668761603,-4.2113002426,-0.1846244166\H,-6.2876605075,-4.0458590981,-4.2870971722\H,-7.9160641649,-4.8899313291,-2.5824233747\H,-0.4517777554,3.8696604259,-4.6463906099\O,-5.1454001221,5.0535981476,2.8459849176\C,-5.3028283469,5.4306291798,4.2231584146\H,-4.541860781,6.1749877366,4.5197156597\H,-6.3046726179,5.8782880542,4.295626375\H,-5.2432539788,4.5486995642,4.8865265537\\Version=ES64L-G09RevD.01\\State=1-A\\HF=-4089.0593196\\RMSD=5.278e-09\\RMSF=2.596e-06\\Dipole=-3.0915889,5.0495288,4.8014437\\Quadrupole=-14.6266977,12.9159746,1.7107231,-13.5528362,-8.0529718,10.6130341\\PG=C01 [X(C71H56N1O5P1Si2)]\\@

TiPSY/6 Type II Z

1\\GINC-WORKER\\FOpt\\RTPSSTPSS\\def2svp\\W06\\C71H56N1O5P1Si2\\JHIOE\\15-No v-2015\\0\\#p tpsstps/def2svp/w06 densityfit empiricaldispersion=gd3 o pt scrf=(smd,solvent=ch2cl2,read)\\title\\0,1\\P,0.8036362744,0.265906907,1.7183314518\\O,2.0458581008,1.3086247906,1.3117850366\\O,-0.3537906388,0.7503950095,0.5519240536\\O,0.3967815805,0.6008241241,3.1203883892\\O,1.1784892938,-1.1407954917,1.25153993\\C,1.6717900163,2.1162117362,-0.8759321809\\C,2.4410367222,1.3342050263,-0.0124906439\\C,3.5939685133,0.5945496353,-0.4178659413\\C,3.9465792771,0.677549226,-1.7638164988\\H,4.82883174,0.143299571,-2.1360351358\\C,3.1754863023,1.4094499967,-2.7135887402\\C,2.0041888323,2.1294983379,-2.2765902541\\C,1.1969635985,2.7718229893,-3.2642466902\\H,0.2835567716,3.2882462422,-2.9561767932\\C,1.5453365131,2.7316597404,-4.6066132232\\H,0.9056206626,3.224039588,-5.3472242902\\C,2.7177652099,2.0497372254,-5.0316642468\\H,2.9815806682,2.0291556741,-6.0945826529\\C,3.5123814481,1.3994419665,-4.1011392943\\H,4.4071399703,0.8510785635,-4.4169213124\\C,0.474095066,2.8260323215,-0.34134

91487\C,-0.5480447415,2.0917469055,0.2780312882\C,-1.8442701786,2.6443
838346,0.535093016\C,-2.0021314341,4.0167767378,0.3516010904\H,-2.9750
165939,4.4857804312,0.5373135355\C,-0.9390007278,4.8534968969,-0.09687
54517\C,0.3122190094,4.2500368744,-0.4795022535\C,1.3571461517,5.09967
54181,-0.9531280352\H,2.3205181886,4.6584585465,-1.2261134186\C,1.1708
821525,6.4708783755,-1.0519647473\H,1.9899334424,7.1050712387,-1.40884
91472\C,-0.0689942172,7.0624643271,-0.6881190699\H,-0.2022236998,8.146
2756618,-0.7751367919\C,-1.1012287552,6.266099045,-0.2172725125\H,-2.0
612700218,6.7091141592,0.0716462918\C,-5.1847022658,-4.5566304926,-1.0
188323297\C,-4.5870831148,-3.4081127343,-1.5943287023\H,-5.1319007172,
-2.8666320265,-2.3720965231\C,-3.344508527,-2.9698698276,-1.1615785657
\H,-2.9251605823,-2.0604457978,-1.5999414377\C,-2.6510086975,-3.654427
1306,-0.1250628476\C,-3.2765860316,-4.7795823347,0.4640620333\H,-2.776
4905004,-5.3230663177,1.2707950139\C,-4.5161721203,-5.2434380258,0.019
9357329\H,-4.9548258111,-6.1295674747,0.4845721794\C,-1.3885041916,-3.
1528803611,0.4160341553\C,-1.079611219,-3.3496452556,1.8709794801\H,-0
.2117751324,-2.7452294571,2.172923649\H,-0.8412204673,-4.4168249935,2.
0411294927\H,-1.9550752223,-3.0992279958,2.4897180795\N,-0.4843020443,
-2.4937342129,-0.2851541235\H,0.2536385379,-1.9736555564,0.3035626988\
C,-0.3197629317,-2.3548949925,-1.6937442208\C,0.2334752097,-1.15108240
14,-2.1678531483\H,0.4532087669,-0.3463130575,-1.4612891665\C,0.493839
08,-1.0011659324,-3.5363950415\H,0.9187137762,-0.0613219924,-3.9013128
117\C,0.2115910823,-2.0460635431,-4.4289680428\C,-0.3210704197,-3.2536
641675,-3.9448488053\H,-0.5221985694,-4.0817196874,-4.6327752573\C,-0.
5812269327,-3.4186339843,-2.579861505\H,-0.9670324014,-4.36837522,-2.2
002426167\H,0.4169147434,-1.9259450876,-5.4978607773\Si,-3.4067504063,
1.5663835713,0.6874801559\Si,4.5776672492,-0.572893934,0.7282360841\C,
6.4270386558,-0.3636636528,0.3071776067\C,7.2984103032,0.4656892889,1.
0505812902\C,6.9701139351,-1.0535688429,-0.8048032282\C,8.6488117609,0.
6108637228,0.6935070351\H,6.9263270642,1.0029769692,1.9302324957\C,8.
3177212155,-0.9082849542,-1.1696278289\H,6.3323082397,-1.7253368215,-1.
3926123229\C,9.16133474,-0.0730439957,-0.420213116\H,9.3031782942,1.2
573857352,1.289596138\H,8.7110040528,-1.4536581653,-2.0353246421\H,10.
2153880192,0.0389318665,-0.6986901817\C,4.1566110058,-2.3711026584,0.3
039248263\C,3.1502611097,-2.7131705887,-0.6244908014\C,4.8802620967,-3.
4242082137,0.9133887053\C,2.8645310355,-4.053596438,-0.9275457906\H,2.
5748101551,-1.9210285524,-1.1125691599\C,4.5936074897,-4.7669660321,0.
6212485845\H,5.681464528,-3.1970082538,1.6279508142\C,3.5824203728,-5.
0845516244,-0.3005813429\H,2.0766846521,-4.2903673299,-1.6515423179\H
,5.1624886031,-5.5660391483,1.1104484946\H,3.358464447,-6.1322295173,-
0.5320431549\C,4.291109556,-0.2058720658,2.5620013951\C,3.8330269409,-
1.2012409493,3.4526627507\C,4.4842888918,1.099811126,3.0729426612\C,3.
5809454762,-0.9072841407,4.8029451343\H,3.6476182188,-2.2170973803,3.0
867769593\C,4.2363794311,1.3980923683,4.4197087789\H,4.8040372021,1.90
75822846,2.4036762124\C,3.783093182,0.3925442186,5.2897565245\H,3.2163
908431,-1.6945211153,5.4728385559\H,4.3851626962,2.4192305278,4.789188
2083\H,3.5801264202,0.6253129767,6.3413646255\C,-3.7534318802,0.869726
1006,-1.047003476\C,-5.0673841092,0.4843551074,-1.4092881507\C,-2.7369
336075,0.7280262727,-2.019472338\C,-5.3517626039,-0.0261517439,-2.6852
100993\H,-5.8872577007,0.5935647521,-0.6891818176\C,-3.0151271501,0.21
37421824,-3.2959044758\H,-1.7083493024,1.0199708427,-1.7848036216\C,-4.
3240425103,-0.1651723332,-3.6321476693\H,-6.37713691,-0.3170627829,-2.
9400297364\H,-2.2057337486,0.1080077411,-4.0264146651\H,-4.5431858693
, -0.5663348129,-4.6280510902\C,-4.8477992875,2.7217902871,1.1454169184
\C,-5.5045928787,3.5045966893,0.1654248119\C,-5.2691821669,2.858018102
8,2.4884417153\C,-6.5369576457,4.3898141898,0.5128525468\H,-5.20610486

47,3.422582273,-0.8867588422\C,-6.3002320424,3.743136412,2.8415919541\H,-4.7873126413,2.2629402378,3.2737106677\C,-6.9368514459,4.5110059386,1.8536210833\H,-7.0312342586,4.984528997,-0.2638734863\H,-6.6091903437,3.8308695903,3.8895555755\H,-7.7439159049,5.2002168563,2.1270545611\C,-3.3909835658,0.1887335095,1.9814456329\C,-2.6424588996,0.3058419011,3.1733397654\C,-4.2584394434,-0.9216750084,1.8457891596\C,-2.7650143212,-0.6448676931,4.1993372101\H,-1.9329136821,1.1291798789,3.2957929405\C,-4.3881203606,-1.8702419386,2.8716071725\H,-4.842099499,-1.0548957653,0.927570854\C,-3.64550173,-1.7285661634,4.0562452729\H,-2.1626330493,-0.5404253224,5.1087510657\H,-5.0632325255,-2.7237781824,2.742250802\H,-3.7419518765,-2.4696942989,4.8578558282\O,-6.3877826363,-4.9055294092,-1.5178112161\C,-7.0727540752,-6.0445097521,-0.9710656249\H,-8.0144044587,-6.1204567605,-1.5340805933\H,-6.4814495465,-6.9676208846,-1.1099880644\H,-7.2927927288,-5.8966708632,0.1017220795\\Version=ES64L-G09RevD.01\\State=1-A\\HF=-4089.0624805\\RMSD=4.962e-09\\RMSF=4.191e-06\\Dipole=-4.1466294,-4.7112296,-3.4343391\\Quadrupole=0.6755835,23.1820437,-23.8576271,34.5447013,-7.9584256,-4.4817681\\PG=C01 [X(C71H56N1O5P1Si2)]\\@

TiPSY/7 Type I E

1\\GINC-LOGIN\\FOpt\\RTPSSTPSS\\def2SVP/W06\\C71H53F3N1O4P1Si2\\JHIOE\\15-Nov-2015\\0\\#p tpsstpss/def2svp/w06 densityfit empiricaldispersion=gd3
opt scr=(smd,solvent=ch2cl2,read)\\title\\0,1\\P,0.3014353525,-0.5497520906,-1.431257563\\O,-0.9499440114,0.5427685516,-1.6993063089\\O,1.2112678277,0.2788424359,-0.2619516967\\O,1.0175905469,-0.6743197114,-2.7424792498\\O,-0.2237964717,-1.7412289197,-0.6475216795\\C,-0.7537158599,2.3046376891,-0.0821949946\\C,-1.5165301831,1.3111157578,-0.7012917839\\C,-2.9121092397,1.1244532297,-0.4510939142\\C,-3.5044538402,1.9195942839,0.5241445972\\H,-4.5724817485,1.8151717661,0.7425465635\\C,-2.7555332136,2.8628573173,1.2869276841\\C,-1.3555344215,3.051349792,0.9983764847\\C,-0.6137638539,3.9495111397,1.8239869871\\H,0.4584700391,4.0758655884,1.6486912306\\C,-1.2283012039,4.6458022994,2.8549312827\\H,-0.6342583681,5.3204000586,3.4814076197\\C,-2.6160707065,4.4862141017,3.1123073701\\H,-3.0880616336,5.0448609398,3.927716319\\C,-3.3605599018,3.6059139197,2.3439699403\\H,-4.4243822549,3.4457346788,2.550821219\\C,0.6437897092,2.588747198,-0.5142532428\\C,1.6131270099,1.580640665,-0.4945848462\\C,3.0160052413,1.8473075262,-0.5944139858\\C,3.3966061973,3.1537512403,-0.8936103778\\H,4.4591295132,3.4153963321,-0.9565644261\\C,2.4441297414,4.1881856035,-1.1260714362\\C,1.0441910249,3.9120872659,-0.9241746903\\C,0.1062897513,4.9599348518,-1.1698661918\\H,-0.9626230226,4.757764629,-1.0542628007\\C,0.5313663165,6.217384647,-1.5733181178\\H,-0.207875477,7.0022750654,-1.7680214108\\C,1.9144392085,6.4959205658,-1.7432946709\\H,2.2348481348,7.4959709831,-2.0550343551\\C,2.8501499079,5.497271436,-1.5245105894\\H,3.9197239171,5.6934473186,-1.662171956\\C,-2.540117745,-0.8705222366,3.7014376916\\C,-2.5104045736,-2.1919695451,4.1728311228\\H,-3.2701191591,-2.5433116181,4.8758272613\\C,-1.5085757542,-3.0609024602,3.7316303457\\H,-1.5029793668,-4.093674059,4.090435101\\C,-0.5541942024,-2.6252675264,2.7855701871\\C,-0.5749342674,-1.2822268073,2.3431219857\\H,0.1815694973,-0.913537143,1.6475978523\\C,-1.5599855178,-0.4085712443,2.8048979849\\H,-1.5740772815,0.6267987025,2.453942721\\C,0.4175993653,-3.5996373974,2.2450309958\\C,0.9370253246,-4.6931530301,3.126255513\\H,1.9121280096,-5.0644055116,2.7770122523\\H,0.2289177299,-5.5425054226,3.1281062562\\H,1.0236932601,-4.3276487144,4.1604178146\\N,0.770461448,-3.4693185854,0.9898552583\\H,0.3392701104,-2.667633193,0.3853545384\\C,1.6397773705,-4.2923440632,0.214512875\\C,2.5252489601,-3.6342031364,-0.6612714904\\H,2.5569917587,-2.5431487248,-0.6870026127\\C,3.3768841559,-4.388400

9602,-1.4755422214\H,4.0735220017,-3.8711843375,-2.1422520216\C,3.3317
355809,-5.7914311894,-1.4375824514\C,2.4221366582,-6.4410044931,-0.587
7816849\H,2.3645664703,-7.5343894541,-0.5740776974\C,1.5693755914,-5.6
982095645,0.2393577438\H,0.8336024445,-6.2049227197,0.8682550702\H,3.9
960478058,-6.3784351647,-2.0805077765\C,-3.6565187203,0.0567152712,4.1
125234152\Si,-3.9184420549,-0.1165585757,-1.4792911522\C,-3.3395174688
,-1.8885781502,-1.167449372\C,-3.3396031414,-2.3985929019,0.1520497084
\C,-2.8813173053,-2.7316211554,-2.2032793811\C,-2.9159627542,-3.708023
4192,0.4216676075\H,-3.6603280492,-1.7632985414,0.9867554271\C,-2.4425
013115,-4.0374077793,-1.9359552448\H,-2.8476872734,-2.3610118321,-3.23
44407788\C,-2.4621388745,-4.5297077165,-0.6225237272\H,-2.9324633072,-
4.0830171843,1.4505148188\H,-2.0782510357,-4.6691383493,-2.7543180237\H,
-2.1200123045,-5.5496528247,-0.4113569404\C,-5.7368076079,0.06973139
77,-0.9464144654\C,-6.4453802591,-0.9175557648,-0.2259767561\C,-6.4253
091366,1.2618188933,-1.2814015925\C,-7.7826406236,-0.7208229382,0.1569
848757\H,-5.9522763812,-1.8597423668,0.0384908029\C,-7.7598688023,1.46
49252594,-0.8999515105\H,-5.9095173184,2.0460624889,-1.8501093227\C,-8
.4417927005,0.4722244034,-0.1763692234\H,-8.3104079575,-1.5028078848,0
.7150623736\H,-8.2703866866,2.3967991164,-1.16905351\H,-9.4850100699,0
.6273378091,0.1217173006\C,-3.8518435569,0.3383675999,-3.3176852153\C,
-4.6119821846,-0.4203836801,-4.2407302522\C,-3.1262103932,1.4454415391
,-3.8119463871\C,-4.6319984485,-0.0977701235,-5.6061136514\H,-5.202145
2761,-1.2761934432,-3.8887992977\C,-3.1490925927,1.7768274394,-5.17634
15558\H,-2.5327381664,2.0607001173,-3.1269703578\C,-3.8982093693,1.003
4877016,-6.0769385189\H,-5.2234982878,-0.702925355,-6.3027515293\H,-2.
5780538437,2.640297082,-5.5364443453\H,-3.913235898,1.2594972973,-7.14
24529051\Si,4.3343583034,0.5653718036,-0.09578518\C,3.7358814711,-0.36
76301038,1.4424848704\C,4.1167859855,-1.7036267265,1.6984277411\C,2.93
06995143,0.2869277546,2.4052148377\C,3.7084553616,-2.3642348835,2.8686
205137\H,4.7343473292,-2.2451628162,0.972972771\C,2.5248087743,-0.3665
657755,3.5780384375\H,2.6045390656,1.3200350517,2.2337100771\C,2.91371
30372,-1.6956413622,3.8125676043\H,4.0097009375,-3.4035755012,3.040389
6398\H,1.8934881448,0.1572672623,4.3044460733\H,2.5926103495,-2.208814
8913,4.7257904835\C,5.8819808147,1.5613436477,0.3908422571\C,6.1034307
798,1.9814000283,1.722642927\C,6.8230229431,1.9545909804,-0.590977641\H,
7.2154367296,2.7689246241,2.060924799\H,5.3999173038,1.6885610894,2.
5114674269\C,7.9348999977,2.7443557623,-0.2585919617\H,6.6859856988,1.
6392982166,-1.6327083067\C,8.1327272183,3.1539214254,1.0700030001\H,7.
3674748263,3.081238401,3.1005522187\H,8.6487470523,3.0384019001,-1.036
6000804\H,9.0009954822,3.7688984674,1.332824834\C,4.8559406657,-0.5914
792921,-1.4983773538\C,6.0488193165,-1.3465227179,-1.3720210851\C,4.13
49340021,-0.6864424178,-2.7093589602\C,6.5030499335,-2.1666798043,-2.4
157284921\H,6.6421599536,-1.2833421889,-0.4514315264\C,4.5897641566,-1
.5049325664,-3.7567506784\H,3.191387779,-0.1455140338,-2.8331536605\C,
5.7749131336,-2.243216677,-3.6151884239\H,7.4288033161,-2.7409854843,-
2.2961571083\H,4.0105390797,-1.5671435184,-4.6851012999\H,6.129866861,
-2.8793091919,-4.4340257812\F,-3.1945232699,1.2715174617,4.5034217592\H,
-4.5183018989,0.2836868275,3.0783851123\F,-4.3971006902,-0.436007737
2,5.1334602186\\Version=ES64L-G09RevD.01\\State=1-A\\HF=-4311.4204564\\RM
SD=3.937e-09\\RMSF=1.864e-06\\Dipole=1.2431025,-3.9895733,4.3433036\\Quad
rupole=-18.1773123,34.5616125,-16.3843001,-7.2414788,-4.1105377,-22.42
84811\\PG=C01 [X(C71H53F3N1O4P1Si2)]\\@

TiPSY/7 Type II E

1\1\GINC-WORKER1\FOpt\RTPSSTPSS\def2SVP/W06\C71H53F3N1O4P1Si2\JHIOE\01
-Dec-2016\0\\#p opt scrf=(smd,solvent=ch2cl2,read) tpsstpss/def2svp/w0

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798337606\\O,0.7870020741,1.0273125512,0.4160778254\\C,1.2219594381,-2.6
21190017,-0.5872190572\\C,1.9010794256,-1.4292625709,-0.8475074078\\C,3.
1856733206,-1.1089007818,-0.3217467484\\C,3.7716677765,-2.050000359,0.5
229496842\\H,4.7525121023,-1.8513947084,0.9727119302\\C,3.1214377772,-3.
2694825595,0.8718465007\\C,1.8207683487,-3.5654233669,0.3215732333\\C,1.
1561534123,-4.7504074932,0.7620944353\\H,0.1529699465,-4.9725479273,0.3
879521372\\C,1.7557728568,-5.6100631178,1.671293378\\H,1.222283553,-6.50
89051654,1.9996389744\\C,3.0499728818,-5.3318693353,2.188321386\\H,3.511
6005909,-6.0213218072,2.9034137292\\C,3.7144914577,-4.1807667204,1.7970
077467\\H,4.7042891473,-3.9419621189,2.2022520022\\C,-0.1353379842,-2.83
54093994,-1.1683445567\\C,-1.1593222133,-1.9167883009,-0.8998281633\\C,-
2.5346831845,-2.1773761876,-1.2000720138\\C,-2.8284988843,-3.3280817237
,-1.9266484616\\H,-3.8696783957,-3.5772659862,-2.1633148209\\C,-1.810330
9967,-4.2174282621,-2.3797559963\\C,-0.4430643812,-3.980486015,-1.98662
77102\\C,0.5592633363,-4.8856825579,-2.4503509033\\H,1.6048732702,-4.706
7820467,-2.1822360386\\C,0.2269769055,-5.9719454625,-3.2467366471\\H,1.0
148286972,-6.6471656447,-3.5985669578\\C,-1.1234534499,-6.2139614318,-3
.6170547266\\H,-1.3711374029,-7.077719102,-4.2435574542\\C,-2.1196886908
,-5.3495711347,-3.1912689703\\H,-3.1647497401,-5.5175591553,-3.47585808
92\\C,-1.6391144543,5.055108801,-0.0613843578\\C,-1.1901750539,5.5877842
209,1.1624516958\\H,-1.0280997206,6.66467913,1.268466209\\C,-0.937037513
6,4.7350750978,2.2389832178\\H,-0.5681315687,5.148928332,3.1820121079\\C
,-1.1080432534,3.3387168319,2.0906456657\\C,-1.6017061862,2.8261056747,
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.0793817216\\C,1.3995571922,-2.0168591815,4.9458184175\\C,1.3290051615,-
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.8283034839,0.35237457,4.9577560181\\H,0.826787382,1.3119729591,5.47571
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152237969\\C,6.4251667469,1.1382238999,-2.2783511577\\C,6.0880765075,-1.
2402161192,-1.9679781373\\C,7.5682279451,0.8803292898,-3.0502797469\\H,6
.1165576075,2.1789883388,-2.1181995799\\C,7.2281684465,-1.5040287679,-2
.7445872312\\H,5.5184813136,-2.0834058085,-1.5602144748\\C,7.972422924,-
0.4441325653,-3.2854799547\\H,8.1409322843,1.7132710963,-3.4740942399\\H
,7.5331978017,-2.5402826626,-2.9305680746\\H,8.8614636383,-0.6486494682
,-3.8928574507\\C,4.6926024571,1.1228240655,1.0544615716\\C,3.748857683,
1.1621215554,2.1097415067\\C,6.0056189412,1.5712015899,1.3208041611\\C,4
.1031291425,1.6384143269,3.3807392038\\H,2.7248544652,0.8187748291,1.92
53350966\\C,6.364962073,2.046109864,2.5934174725\\H,6.7626352912,1.54683
21331,0.5275901683\\C,5.4138580485,2.0815098501,3.6253379586\\H,3.355765
7711,1.6584486419,4.182102032\\H,7.3901800164,2.3863652772,2.7796046702
\\H,5.6937367545,2.4503415903,4.6187747799\\C,3.2260649932,1.9034165709,
-1.5504082242\\C,2.7828862522,3.0550311694,-0.8631195548\\C,2.9849979344
,1.8300987701,-2.9421567002\\C,2.1086331074,4.0870162102,-1.5339719741\\

H,2.9509864635,3.1421144875,0.2156636255\C,2.3114201767,2.8582035917,-3.6174884714\H,3.3180184035,0.9512079275,-3.5073423945\C,1.8658650347,3.9884187975,-2.9123981362\H,1.7581407185,4.9642135494,-0.9790978435\H,2.1245473042,2.7737897624,-4.6943062539\H,1.3232977058,4.7865111133,-3.4315906763\C,-5.5211062245,-2.15631105,-0.5650852819\C,-5.9496425005,-3.0477610756,0.4451944279\C,-6.3047147662,-2.0661508995,-1.7406593748\C,-7.1102646462,-3.8223598422,0.2875199618\H,-5.373394822,-3.1385715038,1.373811319\C,-7.4648820099,-2.8392875114,-1.9042095632\H,-6.0060512856,-1.3796870742,-2.5426574688\C,-7.8698512153,-3.7206987648,-0.8888895919\H,-7.4236133049,-4.5047618838,1.0860531461\H,-8.054571246,-2.7514823964,-2.8239972913\H,-8.7765028497,-4.3238754174,-1.0125400992\C,-4.2478472613,0.5049810084,-1.284730707\C,-3.494579355,0.9362448913,-2.3978676191\C,-5.3289843746,1.316509613,-0.8581538918\C,-3.7963397715,2.1435497834,-3.0499283427\H,-2.6440577333,0.3438569816,-2.7458297776\C,-5.6269180707,2.5266694658,-1.5012429239\H,-5.9559770246,0.9962018336,-0.0166853162\C,-4.857601743,2.9436689081,-2.6005675007\H,-3.1862021028,2.4679994325,-3.9002578662\H,-6.4622393554,3.142291066,-1.1482434881\H,-5.081531135,3.8923708412,-3.1008779171\C,-3.5239594434,-0.9292863343,1.4322825367\C,-2.9729768894,-2.0190389784,2.1495227299\C,-3.801259231,0.2564130175,2.1485202803\C,-2.7187080279,-1.9314172768,3.526376338\H,-2.7266187446,-2.9502924007,1.6241586159\C,-3.5409546556,0.3512859627,3.5255400715\H,-4.2173562283,1.1271634744,1.6300037232\C,-3.0019422999,-0.7431552243,4.2189986671\H,-2.2842571136,-2.7855208205,4.0573703051\H,-3.7595483692,1.2842182459,4.0566801253\H,-2.7937313924,-0.6693451897,5.292243433\F,-2.4408124758,7.1349530679,-0.893878155\F,-0.6199400712,6.3357332585,-1.7831224188\F,-2.5459154148,5.4169151178,-2.2378030911\\Version=ES64L-G09RevD.01\\State=1-A\\HF=-4311.4211313\\RMSD=2.448e-09\\RMSF=3.683e-06\\Dipole=-0.4400647,-0.0768842,6.4076198\\Quadrupole=-17.744294,-0.9705873,18.7148812,-5.0472614,1.3271282,24.507198\\PG=C01 [X(C71H53F3N1O4P1Si2)]\\@

TiPSY/7 Type I Z

1\\GINC-LOGIN\FOpt\RTPSSTPSS\def2SVP/W06\C71H53F3N1O4P1Si2\JHIOE\19-Nov-2015\\#p tpsstps/def2svp/w06 densityfit empiricaldispersion=gd3
opt scrf=(smd,solvent=ch2cl2,read)\\title\\0,1P,0.6627458837,-0.5160601969,-1.6514951178\O,1.6856521963,-1.7140025338,-1.0866181981\O,-0.6059023003,-0.6746404539,-0.5188174967\O,0.2677745405,-0.9031792609,-3.0418935088\O,1.2683775726,0.8415586269,-1.2879073584\C,1.0454234968,-2.2732899616,1.1208354421\C,1.991672095,-1.7100446659,0.2612866225\C,3.2381271988,-1.1599294736,0.6972502773\C,3.5073894607,-1.2296579865,2.0631794062\H,4.4571384423,-0.84921318,2.4568088391\C,2.5661519006,-1.7412629865,3.0042980736\C,1.2972708417,-2.244799172,2.5382580912\C,0.3293212869,-2.6420423146,3.5102291076\H,-0.6539471462,-2.9856981777,3.176628836\C,0.6146143874,-2.5832888032,4.866546008\H,-0.1462674399,-2.8871162201,5.5938999626\C,1.8820241527,-2.1295256443,5.3222480208\H,2.0957378243,-2.0975763154,6.3961180924\C,2.8349916015,-1.7132653183,4.4066248559\H,3.8085013612,-1.3399495436,4.7448223116\C,-0.2364488137,-2.7901455412,0.5605064641\C,-1.066481252,-1.9327727361,-0.1762516859\C,-2.4237724546,-2.2593214937,-0.496962385\C,-2.8529249911,-3.555667811,-0.2210016316\H,-3.88467023,-3.8504252691,-0.4454440516\C,-1.9975123389,-4.5318410717,0.368848108\C,-0.6756061134,-4.1423489972,0.7904008932\C,0.1599994611,-5.1287629696,1.3959012156\H,1.1749432583,-4.8551651536,1.6990482838\C,-0.291623595,-6.4265583045,1.5856128848\H,0.3706514416,-7.1693989007,2.0437849124\C,-1.6013325079,-6.8045898944,1.1844706876\H,-1.9450631434,-7.8324274042,1.3436811375\C,-2.434589507,-5.8731542655,0.5848090695\H,-3.4446543026,-6.1524485344,0.2635479491\C,-3.579282538

1,4.4445379399,3.274113593\C,-3.6396295534,4.1689862011,1.8964374146\H
,-4.5152351,4.4639822774,1.3116209455\C,-2.5794662456,3.5088629457,1.2
759575696\H,-2.6318999928,3.2809635322,0.2086176043\C,-1.4567716122,3.
10017695,2.0306145327\C,-1.4193050696,3.3533652389,3.4173566043\H,-0.5
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036783\H,-2.4319740674,4.2518536023,5.1059864339\C,-0.3917256712,2.309
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089\H,0.7731816827,1.4420583061,2.9202864669\N,0.0792110635,2.60095524
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\H,2.6741453245,3.8816548451,1.9331709116\H,5.0874172498,4.6795418266,
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2.6281472203,-3.8773946125\H,4.7155774474,-2.8648388424,-1.7843510803\
C,3.8601075882,-1.7474516117,-4.8963184834\H,3.3130265197,0.2955904571
,-5.3818362928\H,4.4144832024,-3.6904452667,-4.0979667475\H,3.70810899
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,1.8614682611\C,-5.577400363,1.3643253999,2.1313417853\H,-5.9298361519
,0.9085961249,0.0518240517\C,-4.7596181897,1.157004165,3.2542804768\H,
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2092756994\H,-4.9995541255,1.6461616138,4.2034899006\C,-5.3044481018,
-1.8154770249,-1.4603587025\C,-6.2389573308,-2.3208697122,-0.524953991
6\C,-5.5611758254,-2.0350414089,-2.8336865639\C,-7.3807496506,-3.02241
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-3.4043376993,-0.2003115224\H,-6.8786062973,-2.8941621006,-4.327126793
 \H,-8.5040520966,-3.7796509144,-2.6414616609\H,-0.3162393946,4.6781982
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 53F3N1O4P1Si2)]\@

TiPSY/7 Type II Z

1\1\GINC-LOGIN\FOpt\RTPSSTPSS\def2SVP/W06\C71H53F3N1O4P1Si2\JHIOE\15-N
 ov-2015\0\#p tpsstps/def2svp/w06 densityfit empiricaldispersion=gd3
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 1,1.004007325,0.5242135278\O,0.7820266833,0.9654412667,3.0753003679\O,
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 0808257809\C,2.7812454598,1.1541466148,-0.1654250712\C,3.8103642808,0.
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TRIFP/5 Type I E

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TRIFP/5 Type II E

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TRIFP/5 Type I Z

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TRIFP/5 Type II Z

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TRIFP/6 Type I E

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TRIFP/6 Type II E

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TRIFP/6 Type I Z

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TRIFP/6 Type II Z

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TRIFP/7 Type I E

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TRIFP/7 Type II E

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TRIFP/7 Type I Z

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2.2653110241,1.2875828962,-3.6128442726\H,2.3230345364,0.3332683799,-4
.1422339842\C,2.2401084632,1.429196156,2.0908968109\C,1.6434634554,2.6
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4113\C,3.626752272,3.5491216542,0.8290616639\C,-4.5083671104,-0.812734
5342,-0.2195965901\C,-4.8779027206,-0.958957879,-1.5714494565\C,-5.143
3059835,0.1902920765,0.5439889767\C,-5.8543257249,-0.1286831892,-2.141
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0.3219602507,1.5956977823\H,4.157664905,4.364169403,0.3315952464\H,4.0
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33513\F,-6.0612174212,3.3004893126,0.626954183\F,-6.7388409799,1.84976
94406,2.1047365666\F,-7.2000269241,-1.3351376414,-3.6867256485\F,-5.21
55413503,-0.7349842419,-4.3523302186\F,-6.7978989771,0.7569576322,-4.1
420316949\F,1.1845632084,5.530701088,2.4142785659\F,0.5843846054,5.022
6239049,0.3859263523\F,2.4793211135,6.0461554848,0.7322042055\F,6.3977
819389,3.0534007992,0.3983903861\F,5.357033527,1.8534424455,-1.0930485

938\F,6.1468101374,0.9047651105,0.7060336672\F,6.8449011003,-2.8738638
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3791,-2.8525832546,-3.5568243784\\Version=ES64L-G09RevD.01\\State=1-A\\H
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87,-2.218004\\Quadrupole=-27.8627674,9.2414258,18.6213416,23.2639738,1.
3126074,-7.8439437\\PG=C01 [X(C51H29F15N1O4P1)]\\@

TRIFP/7 Type II Z

1\\1\\GINC-LOGIN\\FOpt\\RTPSSTPSS\\def2SVP/W06\\C51H29F15N1O4P1\\JHIOE\\14-Nov
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57\\O,-1.2729147511,-1.3798237383,-0.9898523504\\C,-1.487625833,1.770177
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7515,0.4548286299,0.8480180174\\C,-3.8574173906,0.4724217684,2.20318134
94\\H,-4.7778906363,-0.0056373288,2.5544300996\\C,-3.0016947875,1.080690
1515,3.1622490885\\C,-1.7737179905,1.7015969337,2.7302946467\\C,-0.87041
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0141,1.4828189712,6.5648339935\\C,-3.3123103083,1.0326622794,4.55557681
61\\H,-4.2568066126,0.5708766314,4.8641757549\\C,-0.2674416503,2.4495441
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,3.192004312,4.0040315946,-0.2624154895\\C,1.302990304,4.3775427092,0.7
462733227\\C,0.0244267751,3.8247476798,1.1177473561\\C,-0.9102573621,4.6
782947679,1.7790535436\\H,-1.9012548112,4.2913201456,2.0330280617\\C,-0.
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5342026\\C,0.6918096923,6.5190534546,1.7587069988\\H,0.9371989208,7.5551
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66\\C,4.5616904023,-1.2854505141,2.0813445685\\H,4.7216613298,-0.5176036
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, -3.6361484336,0.2750240964\\C,1.769204545,-2.5147833119,-0.1509156022\\
C,1.7225066269,-2.5802185396,-1.6410278799\\H,0.6913562584,-2.557856764
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71134,1.9053445879\\C,-0.5220934622,-1.6366807575,2.4755974527\\H,-1.030
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6353038586,4.6522232076\\C,0.8028221551,-3.541557431,4.0653844212\\H,1.3
042780972,-4.296302579,4.6801093263\\C,1.0586870333,-3.4939353206,2.690
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8705359,-1.2226061749\\C,2.5247208765,0.9928735559,-2.4840832193\\C,4.19
03903837,1.3400506934,-0.7536259727\\C,3.4915026352,0.3359987418,-3.263
1789838\\C,5.1380938338,0.6596166434,-1.530623372\\C,4.799738611,0.15363
49754,-2.7943518837\\C,-4.3971930131,-0.2857418988,-0.1201824253\\C,-4.9
074214239,-1.5536069706,0.2331419091\\C,-4.7233277566,0.2394600132,-1.3
862194958\\C,-5.7214411673,-2.2683570139,-0.65369479\\C,-5.5345757774,-0.
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.2490077603\H,1.499721085,1.0937486296,-2.8577588481\H,5.5419494062,-0.3700660161,-3.4024995368\H,4.4713352199,1.7248344803,0.230386324\H,-4.6511052213,-1.9903509682,1.2020813677\H,-4.352046866,1.221944474,-1.6842919178\H,-6.6764394149,-2.3044018556,-2.6086573466\C,3.09375207,-0.2206927958,-4.6094740316\C,6.5486328005,0.4796068413,-1.026189362\C,-6.2332594336,-3.6391708218,-0.285661933\C,-5.8239109619,0.0897233414,-3.6328827498\F,-6.0989599641,1.4184409168,-3.5709065246\F,-6.8792575186,-0.5097685042,-4.2371267281\F,-4.7624512716,-0.0444136513,-4.4729537373\F,-6.0985612755,-3.9087161879,1.0354756798\F,-7.5493682231,-3.784092661,-0.5918171088\F,-5.5742766693,-4.6226552542,-0.9571364361\F,7.0147977129,-0.7745924579,-1.2644874279\F,6.6525819202,0.6985532234,0.3091508369\F,7.4188977456,1.3324535959,-1.6308716962\F,2.4827920046,-1.4363955799,-4.5029199832\F,4.1615853933,-0.4002108874,-5.4261741616\F,2.2221564494,0.5889043391,-5.2575467015\F,7.9906064105,-2.0045662949,1.3212680441\F,7.2549921057,-2.879084958,3.1750361858\F,7.154452199,-0.7216694891,2.8774697322\\Version=ES64L-G09RevD.01\\State=1-A\\HF=-4153.5710903\\RMSD=4.156e-09\\RMSF=3.460e-06\\Dipole=2.2331952,-1.3467325,4.9989331\\Quadrupole=-24.6556428,24.8476862,-0.1920434,-12.2353224,-23.9544221,7.906713\\PG=C01 [X(C51H29F15N1O4P1)]\\@

TRIM/5 Type I E

1\\1\\GINC-WORKER0\FOpt\RTPSSTPSS\def2SVP\C53H48N1O4P1\\JHIOE\24-Apr-2018
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4445753358,-6.7593282506,-0.0759896243\C,2.488803112,-4.9255523785,0.5
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6078528,-0.5221976421\C,3.8820766371,0.6171273141,-1.7648178795\C,3.81
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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
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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
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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-
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3,-2.6036539,-20.8029182,2.3839022,-6.5868824\PG=C01 [X(C53H48N1O4P1)]
\\@

TRIM/5 Type II E

1\1\GINC-WORKER0\FOpt\RTPSSTPSS\def2SVP\C53H48N1O4P1\JHIOE\19-Feb-2019
\0\#p tpsstps\def2svp empiricaldispersion=gd3 int=ultrafine opt scrf
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.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
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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\
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,-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
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 \C,-3.3065011483,5.3611282579,-1.1392614848\H,-4.354007383,5.646787500
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 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
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 916\H,5.0525639248,-3.3668641124,2.0319307739\C,3.6499755476,-2.027028
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 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
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 (C53H48N1O4P1)]\\@

TRIM/5 Type I Z

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TRIM/5 Type II Z

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TRIM/6 Type I E

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810367965\H,0.0307298516,-5.5121099604,-4.0768082699\C,1.1954095436,-0.9137618717,4.0701372139\C,0.0246214764,-1.2003231266,4.8144312996\H,0.1133585328,-1.8093782857,5.7189168788\C,-1.2076083016,-0.7222384469,4.3918643288\H,-2.0879003473,-0.9683466653,4.990663233\C,-1.3291200889,0.0736648705,3.2159649538\C,-0.1400758996,0.3626619469,2.4958975884\H,-0.1768576077,0.9610526721,1.5818501899\C,1.0991667293,-0.1205991905,2.9019419635\H,1.9826067714,0.1148535823,2.3045058954\C,-2.6389793618,0.5479569834,2.7784996898\C,-3.8698962367,0.1343746486,3.5352146939\H,-4.7818046844,0.2841836702,2.9413176583\H,-3.9600545285,0.7181779264,4.4687347111\H,-3.7982822767,-0.9274611891,3.8136016969\N,-2.7521625212,1.3232191619,1.7090178313\H,-1.9097003663,1.5380892163,1.0939733629\C,-3.9474164388,1.9227407589,1.1981198001\C,-4.2242462095,1.7881674566,-0.175632233\H,-3.5478658221,1.2305787729,-0.8297860179\C,-5.3822436541,2.3757013342,-0.7015704001\H,-5.6029911282,2.2575628,-1.7676864938\C,-6.2521998678,3.1035105962,0.1257908664\C,-5.9522716022,3.2585749923,1.4886812897\H,-6.6134097755,3.8439694554,2.1363876943\C,-4.7984868923,2.6758866156,2.0293805529\H,-4.5479519892,2.8180202491,3.084319208\C,-2.6580022873,-2.2616225989,-1.1857099111\C,-3.6700172801,-1.8176263647,-2.0721547083\C,-2.9529414843,-2.4721991273,0.1870531488\C,-4.9599116215,-1.5716341331,-1.5614153111\C,-4.2554805929,-2.2219600251,0.6517262342\C,-5.2735567736,-1.7585872759,-0.2043727918\H,-5.7362655563,-1.2063223627,-2.2449956682\H,-4.478608705,-2.3864286369,1.7129280897\C,2.6433753772,3.1057340554,-1.1653898519\C,2.2404418196,4.0063620906,-0.1496053383\C,2.8777933388,3.5765670457,-2.4843208157\C,2.0913357539,5.3706030372,-0.4692771137\C,2.7180183995,4.945291414,-2.7591497732\C,2.3266004753,5.8624593815,-1.7644252229\H,1.7763573115,6.0653239788,0.319374509\H,2.9056452613,5.3054381224,-3.7786651395\H,-7.1562815105,3.5589350696,-0.2921933408\C,3.2923379263,2.6196507385,-3.5803614061\H,2.4838786478,1.8968727858,-3.7956292643\C,1.9139055213,3.5116424884,1.2419174573\C,2.1685569608,7.3310845744,-2.0919429525\H,1.8661418643,7.9137048407,-1.2054229117\C,-6.6512068239,-1.4443027221,0.3360359624\H,-7.3452951725,-1.1525791709,-0.4700558648\C,-3.3641694008,-1.5496082348,-3.5290266737\H,-3.0017070162,-2.455166969,-4.047391244\C,-1.8795292508,-2.9470880058,1.142033284\H,-1.0926442168,-2.1813935469,1.2630409973\H,2.7312831516,2.9068599004,1.6716047463\H,3.5259556189,3.1598356749,-4.5129579423\H,4.1807627159,2.0304543783,-3.2883725849\H,3.1142738493,7.7571981315,-2.4758709392\H,1.4063978,7.4843406041,-2.8786645043\H,1.7089528288,4.3527315529,1.9254581534\H,1.0142551049,2.8723008927,1.197320883\H,-7.0840465842,-2.3123340737,0.8668077208\H,-6.6091884476,-0.6109419144,1.0625820815\H,-4.2614862886,-1.1869507477,-4.0587217154\H,-2.5772525368,-0.7783313332,-3.6055267446\H,-2.2998213105,-3.1617480938,2.1386528109\H,-1.3845022168,-3.8624686579,0.7701361645\O,2.3430436161,-1.4305086691,4.5442682813\C,3.5561185559,-1.2248489655,3.7955645002\H,4.338858218,-1.7702208916,4.3419109991\H,3.4568640836,-1.6373852129,2.7781060188\H,3.813716915,-0.151975784,3.7478151179\\Version=ES64L-G09 RevD.01\State=1-A\HF=-2819.7397281\RMSD=6.289e-09\RMSF=3.173e-06\Dipole=-0.6869315,-1.1085044,5.0103655\Quadrupole=19.5586836,-17.6270667,-1.9316169,-11.0830477,-13.8552963,4.7503571\PG=C01 [X(C53H48N1O5P1)]\\@

TRIM/6 Type II E

1\1\GINC-LOGIN\FOpt\RTPSSTPSS\def2SVP\C53H48N1O5P1\JHIOE\23-Aug-2018\0
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 smd,solvent=ch2cl2,read)\title\0,1\P,0.1721866513,-0.5092369302,-1.2
 765519995\O,-1.3746145773,-0.0879275735,-1.7712134355\O,0.3731625788,0
 .6359729087,-0.0334018517\O,1.0869002026,-0.2501124859,-2.438276846\O,
 0.1606286532,-1.8190194287,-0.4954847129\C,-2.3594176932,1.2683961522,

-0.0591452859\C,-2.3573276992,0.0915589601,-0.8151710115\C,-3.35767376
56,-0.9211681064,-0.6859053583\C,-4.3576388574,-0.7305909674,0.2584861
641\H,-5.1466464327,-1.4828386631,0.3663316103\C,-4.3703653297,0.40337
93946,1.1190908183\C,-3.3480375071,1.4117466456,0.980849663\C,-3.32996
04856,2.4849009891,1.9230918801\H,-2.5359221598,3.2345526793,1.8631328
276\C,-4.2880044706,2.5783834356,2.9220693913\H,-4.2450012517,3.405782
5054,3.6388932834\C,-5.3185118613,1.6058042552,3.0296335918\H,-6.07262
33431,1.6943900409,3.8191980997\C,-5.3536098491,0.5393426765,2.1454505
411\H,-6.1281890514,-0.2312201121,2.2313923249\C,-1.3189214841,2.30853
62148,-0.3064407628\C,0.0344939907,1.9542877104,-0.2568603511\C,1.0928
749146,2.9092153931,-0.3554145755\C,0.7525171077,4.239205422,-0.566277
2247\H,1.5440914019,4.9940589642,-0.6291738224\C,-0.6019311725,4.65112
25755,-0.7251330264\C,-1.6592557121,3.676075416,-0.6087655192\C,-3.002
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9664687\C,-3.2899887362,5.4345523055,-1.1165698748\H,-4.3279617563,5.7
393311028,-1.2901851329\C,-2.2499150226,6.3995231021,-1.1954991005\H,-
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1.0079707406\H,-0.1199629078,6.7418832511,-1.0841449758\C,5.507424527,
-1.9799487648,-0.6462756124\C,5.7332383628,-2.6258229325,0.5944301218\H,
6.6974131917,-3.1147274114,0.7628098514\C,4.7422900839,-2.6432061224
,1.5681126908\H,4.9366632098,-3.1704227643,2.5066744942\C,3.4826852619
, -2.0242660031,1.3359490297\C,3.2925557205,-1.3551303864,0.1026124419\H,
2.3864232925,-0.7752134553,-0.0674600762\C,4.2719167401,-1.337346728
9,-0.8842371727\H,4.0715122666,-0.7980083226,-1.8111737752\C,2.4243284
63,-2.085415398,2.3414162675\C,2.7742866739,-2.3043027011,3.7846519632
\H,1.977934921,-1.938747998,4.4503862954\H,3.7182272306,-1.7915913647,
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-1.9316582273,1.9681857686\H,0.9064612267,-1.8290934696,0.9306302545\C
,0.001727325,-1.9543594494,2.8028848173\C,-0.8927014395,-0.8728826818,
2.7090198727\H,-0.6649814518,-0.04195348,2.0361814702\C,-2.0670718269,
-0.8865656019,3.472273435\H,-2.7576357564,-0.040227811,3.4115724831\C,
-2.3628034427,-1.9825228951,4.2986188718\C,-1.4788378274,-3.0713973192
,4.3619940306\H,-1.7140236888,-3.9374693072,4.9895917411\C,-0.29268452
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2.5225718758,2.4890948692,-0.2032310232\C,3.3743850401,2.4405577545,
-1.3377912777\C,3.0301132696,2.1684363662,1.0806741503\C,4.7252924312,
2.0937965683,-1.1593423182\C,4.3888207092,1.8213396146,1.2120583496\C,
5.2558683364,1.7832045236,0.1071756871\H,5.3784805318,2.050638101,-2.0
399869305\H,4.7752711403,1.5679884963,2.2070653175\C,-3.3299635352,-2.
1427305298,-1.5498028955\C,-3.0031768513,-3.4006491678,-0.9835164015\C
, -3.652913974,-2.0434977074,-2.9288657066\C,-3.0129332004,-4.541714293
1,-1.8091690507\C,-3.6524698768,-3.2090170047,-3.7150768991\C,-3.33938
59609,-4.4710042898,-3.1746567406\H,-2.7500227273,-5.5123236608,-1.370
1425324\H,-3.9070801517,-3.1285915472,-4.7794714772\H,-3.2881810658,-1.
9918374869,4.8841754129\C,-3.9892596982,-0.7060132429,-3.5506253105\H
, -3.0978063737,-0.0527692247,-3.5756229508\C,-2.6055070524,-3.51783215
52,0.4719721779\C,-3.3682153457,-5.7100682983,-4.0425864427\H,-2.92788
56083,-6.5783446609,-3.5235583233\C,6.7084647549,1.3895442241,0.258585
2043\H,7.380990023,2.22521971,-0.0120961689\C,2.8251982003,2.691291689
1,-2.7250190876\H,2.3809728092,3.6979452327,-2.8194102899\C,2.12907743
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-3.447520457,-3.292410295,1.1504933405\H,6.939113315,1.0884421568,1.
2942846499\H,6.9626897035,0.5444437974,-0.4063917436\H,2.7045685792,2.
0050800856,3.219639794\H,1.5974993819,3.1456946054,2.3967130111\H,3.61
70198671,2.5926951352,-3.4868774607\H,2.0310678612,1.9545090207,-2.945
8165579\H,-2.8139809684,-5.5526260865,-4.98567673\H,-4.4067123242,-5.9

741113411,-4.3202944694\H,-4.3535512415,-0.8277108726,-4.5845339122\H,
 -4.7641683424,-0.1729857254,-2.9704181282\H,-2.2482280478,-4.535764616
 2,0.7020375143\H,-1.796646866,-2.8033903122,0.69824126\O,6.5324180762,
 -2.0053086115,-1.5234779937\C,6.3558376587,-1.4023631952,-2.8179404671
 \H,6.1447137508,-0.3222126119,-2.7275946868\H,7.3095933798,-1.54939844
 05,-3.3449558872\H,5.5408786769,-1.898673105,-3.3745365358\\Version=ES
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 6\Dipole=2.3402782,-1.2692266,4.1037021\Quadrupole=12.1378309,-8.36077
 78,-3.7770531,-11.5491766,-4.2608599,-16.0409702\PG=C01 [X(C53H48N1O5P
 1)]\@

TRIM/6 Type I Z

1\1\GINC-WORKER0\FOpt\RTPSSTPSS\def2SVP\C53H48N1O4P1\JHIOE\26-Jul-2018
 \0\#p tpsstps\def2svp empiricaldispersion=gd3 int=ultrafine opt scrf
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 ,0.614127009,-0.4737541777\O,-0.6032920756,0.3557444103,-2.950936586\O
 ,-0.930217258,-1.4682031005,-1.0406614122\C,-1.6072258536,1.7747271701
 ,1.1514785431\C,-2.3907532762,0.9133267788,0.3787113357\C,-3.446006128
 1,0.1169148172,0.9233812724\C,-3.6557033344,0.1729748074,2.2957380914\H,
 -4.4681690603,-0.411936594,2.7408164762\C,-2.8321669623,0.9592641972
 ,3.1514969581\C,-1.7830315181,1.7691004903,2.5816113589\C,-0.927589927
 9,2.4889331862,3.4704746785\H,-0.1017634222,3.0757951547,3.0584327498\H,
 -1.1185168863,2.4400050377,4.8436361397\H,-0.443989304,2.9948479147,
 5.5050120556\C,-2.1766996833,1.6720562873,5.4001633756\H,-2.3209993622
 ,1.6477215126,6.4857981823\C,-3.0122625307,0.9445155422,4.5679123213\H
 ,3.8211084355,0.3335342287,4.9846317358\C,-0.5623129576,2.6080756227,
 0.4907001058\C,0.4257540357,1.977207779,-0.2719593086\C,1.5678291966,2
 .6683252869,-0.7825743365\C,1.6384263532,4.042066101,-0.5954234547\H,2
 .5105530334,4.5929654265,-0.9642132462\C,0.6017667416,4.7614690356,0.0
 678751553\C,-0.5188545481,4.0413709944,0.622774083\C,-1.5570940343,4.7
 888708537,1.2572260683\H,-2.4290788024,4.2586508921,1.6517161694\C,-1.
 4814219618,6.1697616662,1.3632108865\H,-2.2940549781,6.7228811052,1.84
 70024004\C,-0.3629718229,6.8744721332,0.8418805781\H,-0.3131792559,7.9
 647753059,0.9361598954\C,0.6539064614,6.1815368838,0.204099413\H,1.514
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 38676\C,4.9710513744,-2.2533041726,2.4520963771\H,5.9413666348,-2.1320
 595609,1.9573478451\C,3.8035874243,-2.1035162904,1.7059059584\H,3.8743
 369168,-1.8492763819,0.6454273506\C,2.5345209757,-2.2279257364,2.32482
 72581\C,2.4828489132,-2.4880906057,3.712820841\H,1.5174053448,-2.57753
 31665,4.2192330536\C,3.6611568124,-2.6642600415,4.4460231295\H,3.59854
 4988,-2.8876845557,5.5167095567\C,1.289601794,-2.0044578777,1.57058475
 88\C,0.1332430703,-1.32384822,2.2394109419\H,-0.6352773219,-1.04041838
 89,1.5073643195\H,0.4795702392,-0.4345740287,2.7893881683\H,-0.3168826
 081,-2.0139269294,2.9773122727\N,1.1363501123,-2.3399067772,0.31093222
 66\H,0.2483906631,-1.9742996317,-0.1974988486\C,1.9901194404,-3.116055
 3046,-0.5334965307\C,2.2450984235,-2.6336089361,-1.8295660933\H,1.8247
 362073,-1.677909186,-2.1527425539\C,3.0580938678,-3.3824223145,-2.6913
 95739\H,3.2689965324,-3.0006447174,-3.6956611479\C,3.5987136306,-4.607
 1362586,-2.2694761201\C,3.3126261359,-5.0935153182,-0.9822806224\H,3.7
 148843706,-6.0586067401,-0.6567224715\C,2.5049581184,-4.354913102,-0.1
 095201495\H,2.2692804865,-4.731912988,0.889599199\C,2.6887335779,1.891
 1750114,-1.400731072\C,2.8410456697,1.8113453196,-2.8051637534\C,3.606
 7263762,1.2326841637,-0.5407317457\C,3.9104845766,1.0568455387,-3.3290
 221326\C,4.6626398419,0.4962142807,-1.1049017307\C,4.8302401702,0.3912
 446582,-2.4997123966\H,4.0238548653,0.9876379485,-4.418106933\H,5.3748

14275,-0.0061570828,-0.4384558324\C,-4.3165334672,-0.7129898771,0.0328
675197\C,-4.2556363193,-2.1298525711,0.0787151121\C,-5.2319563775,-0.0
687524196,-0.8409292485\C,-5.1146783393,-2.8749822757,-0.7513155168\C,
-6.0720392062,-0.8535593764,-1.6512019794\C,-6.0279989213,-2.259783946
4,-1.626114372\H,-5.059945426,-3.9703397563,-0.7173212699\H,-6.7821285
416,-0.3499728454,-2.31928434\H,4.2331579894,-5.1891802442,-2.94615272
76\C,6.2003309209,-2.7372011947,4.6181174878\H,6.848030984,-1.84581034
04,4.529325248\H,5.9979433297,-2.9171435766,5.6864275966\H,6.779615056
6,-3.5932592347,4.22470431\C,-5.3146627956,1.4409614811,-0.9045234415\
H,-4.4101794958,1.8616381246,-1.3809350109\C,-3.2519350809,-2.84336273
07,0.9585239473\C,-6.9117859402,-3.0803130703,-2.5396811853\H,-7.89941
05815,-2.6066274991,-2.6796721883\C,5.9561992796,-0.4373798828,-3.0777
820071\H,6.0400942086,-0.301451055,-4.1692177468\C,1.8492517187,2.4851
701213,-3.726381206\H,1.7646331245,3.565779423,-3.5127312055\C,3.44238
71693,1.3147486851,0.9610899415\H,3.3442609196,2.3620445065,1.29896701
88\H,-3.3673461566,-2.5807811747,2.0244867413\H,4.2988879547,0.8588430
51,1.4832654598\H,2.5265688612,0.7874531023,1.2854071457\H,6.926858270
3,-0.173592423,-2.6197155355\H,5.7909811465,-1.5144289833,-2.883411443
9\H,2.1426782602,2.3638016334,-4.7829859333\H,0.8476232198,2.038066426
7,-3.5869485771\H,-3.352991868,-3.9375679003,0.8621858497\H,-2.2300409
974,-2.5584001925,0.6536652629\H,-7.0657953811,-4.1001457807,-2.146931
0397\H,-6.4531107132,-3.178123456,-3.5429738163\H,-6.1915414699,1.7664
391658,-1.4887730518\H,-5.3846985025,1.8867468348,0.1040466993\\Versio
n=ES64L-G09RevD.01\\State=1-A\\HF=-2744.5683203\\RMSD=2.792e-09\\RMSF=1.53
7e-06\\Dipole=4.0253688,-2.7545032,4.7228696\\Quadrupole=5.6749485,3.162
6588,-8.8376074,-17.3017142,0.7996482,-5.2729635\\PG=C01 [X(C53H48N1O4P
1)]\\@

TRIM/6 Type II Z

1\\GINC-LOGIN\FOpt\RTPSSTPSS\def2SVP\C53H48N1O4P1\\JHIOE\26-Jul-2018\\
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smd,solvent=ch2cl2,read)\\title\\0,1P,-0.8097299545,0.0198445938,-1.5
945530372\O,-2.1085145285,0.9344808595,-1.052246945\O,0.3671978948,0.5
176097658,-0.475648838\O,-0.5186893,0.4696256823,-2.9945337106\O,-1.00
36896992,-1.4509188757,-1.2224842133\C,-1.5749649858,1.7362848631,1.13
56435565\C,-2.3830695381,0.9577767616,0.3025340357\C,-3.5105827685,0.2
17085438,0.7753483372\C,-3.7809370864,0.2493543802,2.1373054442\H,-4.6
468313523,-0.2958476192,2.5282559848\C,-2.9442341304,0.9496777062,3.05
2845913\C,-1.8113368643,1.6930931304,2.5571085168\C,-0.9398044202,2.30
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911936326,2.2240387445,4.8682567912\H,-0.5020425529,2.6960445026,5.577
178377\C,-2.3297758177,1.5251267792,5.3521189045\H,-2.5204817245,1.472
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182749,0.3373693206,4.8204023524\C,-0.4538064189,2.5245452204,0.546572
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215,-0.6410704833\C,1.8703652434,3.8587841917,-0.4023862125\H,2.790265
6826,4.3660265056,-0.7135255294\C,0.8510074624,4.6175092539,0.24362674
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7,6.1043701714,1.5167978622\H,-1.9846999815,6.6886019313,1.99370251\C,
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74124\C,3.6990128986,-2.382970161,1.5112635522\H,2.9449573362,-1.82370
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031493245,-2.3807928333,-1.9327053734\H,1.0793783668,-2.2237135989,-2.
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986418542,-2.1720186175\N,0.9808195457,-2.4564099052,0.1785085768\H,0.
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5516323296\C,-0.08046437,-1.6543428462,2.2036730258\H,-0.3286411148,-0.
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,4.2111391094\C,0.5663461447,-4.0415164428,3.5403963341\H,0.8053461937
,-4.9777435911,4.0557941012\C,0.9586294381,-3.8714071961,2.2068613996\H,
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-1.2195898909\C,3.0475415421,1.5931387508,-2.6177938971\C,3.6841684457
,0.9751525781,-0.3241862073\C,4.0989919581,0.7885358853,-3.0969298415\H,
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,-0.3577735763,-0.1498570115\C,-4.3713129955,-0.5521565352,-0.17706180
07\C,-4.3417993118,-1.9694849787,-0.1770240662\C,-5.2251838776,0.14366
87412,-1.0725581217\C,-5.1730686174,-2.666666411,-1.0747881523\C,-6.04
14115885,-0.5930633484,-1.9487063076\C,-6.0322913922,-2.0008507132,-1.
9663959601\H,-5.1403445819,-3.7633671077,-1.0802684207\H,-6.7028541697
,-0.0514232507,-2.636736043\H,-0.4372695534,-3.1661820005,5.2544659064
\C,7.3636077886,-3.3772266237,1.9810802089\H,7.3013117327,-3.709577191
9,3.032523965\H,7.983186685,-4.0939813299,1.417773804\H,7.8862369604,-
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382541372\C,-6.9377175462,-2.7677761638,-2.9050142348\H,-6.9290774109,
-2.3306381603,-3.9196008744\C,6.0338029153,-0.8276251994,-2.7741591002
\H,6.5118872965,-0.3901356502,-3.6683459761\C,2.1405583371,2.330699242
9,-3.5761803538\H,2.0917702593,3.408367351,-3.3375488361\C,3.471163046
3,1.0751529413,1.1706237596\H,2.5056372865,0.6258852891,1.4672716134\H,
-3.6680421275,-2.5942743021,1.8031722512\H,6.8144010182,-1.022238643,
-2.0190985603\H,5.6141821607,-1.8068015947,-3.0761464337\H,2.490009562
8,2.2225642537,-4.6170448172\H,1.1128261932,1.927955534,-3.5064259858\H,
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5020135874\H,-3.4284451821,-3.8087205765,0.5167437722\H,-2.3732514837,
-2.3653601163,0.6037266124\H,-6.6375628502,-3.8267887841,-2.9808338373
\H,-7.9867425606,-2.7410171958,-2.5518186145\H,-6.0743045744,2.0285387
318,-1.732264665\H,-5.3940202064,2.071014808,-0.0768231227\Version=ES
64L-G09RevD.01\State=1-A\HF=-2744.571283\RMSD=4.930e-09\RMSF=1.426e-06
\Dipole=4.4526636,-3.1427545,3.5680717\Quadrupole=12.8721156,4.3863326
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\\@

TRIM/7 Type I E

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93,0.5088179959,-0.3370009719\O,1.085099841,-0.8532045847,-2.552413411
9\O,0.5116161629,-1.9913100852,-0.2186838212\C,-2.2359909677,0.9947419
917,-0.2624737919\C,-2.2149398761,-0.3357319787,-0.6956251942\C,-3.147
6935694,-1.3194969825,-0.2417433855\C,-4.0893177774,-0.9360846323,0.70
42643154\H,-4.8303991416,-1.6635867222,1.0530805355\C,-4.1105628263,0.
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1715789,3.2117471196\C,0.1642002553,-0.6682876151,2.6298988036\H,0.056
5595624,-1.0799965741,1.6234168856\C,-0.9872895206,-0.2918872395,3.321
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15920379,2.5078824724\C,4.0103062128,-0.5155144199,3.1012345632\H,4.82
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754937\H,3.9675448722,0.5245246914,3.4601148694\N,2.6267752344,-1.5410
160349,1.3644755136\H,1.6956720527,-1.7036460149,0.8510909935\C,3.7376
30717,-2.0743162615,0.6296475869\C,3.8372874363,-1.7822907395,-0.74294
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5748214,-1.4767204748\H,4.9932029798,-2.0708573811,-2.5410767267\C,5.8
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9231959846,1.2555913029\H,4.5538362259,-3.1834905266,2.3115509338\C,2.
5176874858,2.3039547446,-1.1540024716\C,3.264787621,1.9369290056,-2.30
02561817\C,3.1309863033,2.3127900046,0.1262706823\C,4.6154208098,1.567
9932759,-2.1409132541\C,4.4832939145,1.9470763411,0.237913802\C,5.2428
839504,1.5604009402,-0.8834692633\H,5.1869138762,1.2616135037,-3.02594
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19308,-0.8196371528\C,-2.6334717013,-3.7929663869,-0.0654159287\C,-3.6
240910758,-2.9089664823,-2.1346608098\C,-2.639355368,-5.0780745702,-0.
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121,-1.4381883118\C,-2.1244900584,0.691109284,5.351167384\C,-4.1506973
146,-1.7499149338,-2.9521495806\H,-3.3365076379,-1.0452235493,-3.20239
99093\C,-2.0524500915,-3.5868005806,1.3158621008\C,-3.1278678191,-6.69
55497789,-2.547598092\H,-2.642436714,-7.4292059517,-1.8822023565\C,6.6
809941285,1.1197601583,-0.7229030255\H,7.1310488449,0.848428016,-1.692
5614212\C,2.6112531969,1.8743760325,-3.6629300561\H,2.1872507097,2.849
5700731,-3.9613238671\C,2.3354085172,2.6876748906,1.3575382301\H,1.544
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1761287165,-2.3956757212\H,-4.1603988906,-7.0424736433,-2.7416765087\H
,-2.5984523576,-6.7082725367,-3.5181685584\H,-1.7876338192,-4.55070548
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\H,3.3364032053,1.5639042968,-4.4340245833\H,1.7862398287,1.1397916787
,-3.6434603813\H,2.9818558347,2.7451336899,2.2489919456\H,1.8313449474
,3.6630139685,1.2327952098\F,-1.9853221142,0.589860062,6.6968039031\F,

-2.4215933805,1.9930961506,5.0888800929\F,-3.2140146627,-0.0377092597,
5.005257809\Version=ES64L-G09RevD.01\State=1-A\HF=-3042.0902967\RMSE=
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49\PG=C01 [X(C53H45F3N1O4P1)]\@

TRIM/7 Type II E

1\1\GINC-LOGIN\FOpt\RTPSSTPSS\def2SVP\C53H45F3N1O4P1\JHIOE\22-Aug-2018
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,0.601897109,-0.1199973085\O,1.0846632725,-0.2969543508,-2.5482107047\
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3,-0.0605990196\C,-2.2871961458,0.0227260762,-0.7815089779\C,-3.262581
3081,-1.0020918219,-0.5773050589\C,-4.2273145644,-0.7932783385,0.39923
27497\H,-4.99890582,-1.5525090574,0.5666018989\C,-4.222947318,0.369292
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\C,-4.0889124508,2.592192068,2.961902409\H,-4.0258566439,3.4388658127,
3.6543063191\C,-5.105839757,1.6149206765,3.1352611165\H,-5.8285505093,
1.718336894,3.9519605395\C,-5.1652129989,0.5240124952,2.2828434257\H,-
5.9280857698,-0.2506228103,2.4205131385\C,-1.2468623026,2.2607711483,-
0.3701626559\C,0.1090372967,1.9167732199,-0.3473103817\C,1.1605188916,
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37081976,-1.2369653263\C,5.6608376409,-2.7874425826,-0.1000894707\H,6.
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3.5577108895\H,3.4320757455,-3.1741128348,3.7032780176\N,1.3939759046,
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,0.3142902082,-1.8511404682,2.7824219079\C,-0.6379627048,-0.8215491559
,2.6723540052\H,-0.5151474741,-0.0524000745,1.9057552303\C,-1.73376936
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C,-1.8967653278,-1.8306286139,4.4926545398\C,-0.958118499,-2.871674954
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, -1.5674190376\C,-3.5528593719,-3.4195009039,-3.5062451919\C,-3.171040
8216,-4.6445819525,-2.9278002258\H,-2.500590833,-5.5907145311,-1.09945

27063\H,-3.8324398565,-3.3898572323,-4.5669249957\H,-2.7629321306,-1.8
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 6953686,-4.7612946289\H,-4.1893920522,-6.3216848257,-3.856891111\H,-4.
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 ,-2.787667826,0.8404682805\F,6.9534601402,-0.7472456089,-2.4706521443\
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TRIM/7 Type I Z

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 ,0.614127009,-0.4737541777\O,-0.6032920756,0.3557444103,-2.950936586\O
 ,-0.930217258,-1.4682031005,-1.0406614122\C,-1.6072258536,1.7747271701
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 H,-4.4681690603,-0.411936594,2.7408164762\C,-2.8321669623,0.9592641972
 ,3.1514969581\C,-1.7830315181,1.7691004903,2.5816113589\C,-0.927589927
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 ,-3.8211084355,0.3335342287,4.9846317358\C,-0.5623129576,2.6080756227,
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362073,-1.677909186,-2.1527425539\C,3.0580938678,-3.3824223145,-2.6913
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6,-3.5932592347,4.22470431\C,-5.3146627956,1.4409614811,-0.9045234415\H,
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9\H,2.1426782602,2.3638016334,-4.7829859333\H,0.8476232198,2.038066426
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1)]\@

TRIM/7 Type II Z

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176097658,-0.475648838\O,-0.5186893,0.4696256823,-2.9945337106\O,-1.00
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1-Naph/5 Type I E

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877828315,-0.9696257803\C,-3.4459625641,5.829346004,-1.5868446617\H,-3
.9266278873,6.7683130581,-1.8823611072\C,-2.0775241341,5.6684533194,-1
.7355072074\H,-1.4641164914,6.474159499,-2.1545985852\C,-0.0681024081,
-0.9659418194,4.6354732703\C,1.0531931714,-1.7291826074,5.0256989728\H
,1.0948945439,-2.1491083192,6.0367673111\C,2.1158975783,-1.9563836183,
4.1461082795\H,2.9678604574,-2.5553502878,4.4813702725\C,2.0708953698,
-1.4554305421,2.822846037\C,0.9540083126,-0.6788991868,2.4303056366\H,
0.9081184746,-0.2371654002,1.4328065354\C,-0.0852194786,-0.4345276722,
3.3272224066\H,-0.9308823005,0.1808005604,3.0043316955\C,3.1852299829,
-1.7164490609,1.8983166196\C,4.57155535,-1.8833951687,2.4457851229\H,5
.3344672194,-1.6313411188,1.6939157103\H,4.7321632529,-2.9317639586,2.
7574643177\H,4.7001396579,-1.2457698796,3.332967769\N,2.9402096787,-1.
7720809323,0.6072210406\H,1.928522197,-1.6726846389,0.2343703663\C,3.8
694464162,-2.0093876135,-0.4550532889\C,3.7942349231,-1.1738453565,-1.
5855655025\H,3.075560463,-0.3524813431,-1.6211269726\C,4.6596804632,-1
.3968113802,-2.6634056591\H,4.6050890469,-0.7376255281,-3.5357442112\C
,5.584469502,-2.4524430551,-2.6256554308\C,5.6344753716,-3.2980147056,
-1.5061176739\H,6.3374454574,-4.1372215741,-1.479427368\C,4.7757308545
, -3.085680243,-0.419183702\H,4.7872846862,-3.7679642141,0.4348140149\H
,6.2570884507,-2.6240306694,-3.4727423571\C,-1.2284792398,-0.734176120
4,5.5701990907\H,-2.1041599946,-1.326581101,5.2432624045\H,-0.98528005
75,-1.0279095224,6.6045803854\H,-1.5409225004,0.3247293867,5.562786389
\C,-2.6718189657,-2.7431464808,-0.3420613669\C,-1.9782166071,-3.802097
1865,0.3451158367\C,-3.2013163276,-2.9802042992,-1.6086501427\C,-1.334
8577796,-3.6136394721,1.6061236817\C,-1.8898981426,-5.101194494,-0.281
2758987\C,-3.1059840236,-4.2557323007,-2.2213606707\H,-3.71008199,-2.1
66410346,-2.1352712545\C,-0.6657672952,-4.6534685326,2.2325955921\H,-1
.3536691354,-2.6242119536,2.0696819903\C,-1.202886756,-6.1542230116,0.
3973314657\C,-2.4720745273,-5.3001218217,-1.5680353945\H,-3.5440200955
, -4.4090722902,-3.2137243957\C,-0.6063167653,-5.9395075453,1.629308617
\H,-0.1721281575,-4.4797002909,3.1951611436\H,-1.1490716288,-7.1379556
584,-0.0833049584\H,-2.4002335078,-6.2897813912,-2.033488467\H,-0.0787
806421,-6.7553825341,2.1359144438\C,2.0443681681,2.8449237925,-1.48832

92261\C,2.9599994415,2.4840187718,-0.4348721917\C,2.5170864028,2.95882
 4327,-2.7943614295\C,2.5669574832,2.3872821699,0.9341619909\C,4.337733
 3137,2.2108402997,-0.7708943081\C,3.876509805,2.7089821081,-3.11489806
 01\H,1.8138073741,3.2144367887,-3.5938472318\C,3.4692585623,2.00422379
 49,1.914368134\H,1.5333841047,2.6160312374,1.2105028892\C,5.2404965499
 ,1.8114301867,0.2611271453\C,4.7688557019,2.3326894156,-2.1252074603\H
 ,4.2087368378,2.7979133108,-4.1549342196\C,4.8165967878,1.7028809284,1
 .5757707194\H,3.1408449093,1.929299251,2.956585514\H,6.2792998128,1.59
 08453074,-0.0097390175\H,5.815179348,2.1153788382,-2.3672264374\H,5.51
 79594493,1.392154981,2.3576301741\\Version=ES64L-G09RevD.01\State=1-A\
 HF=-2815.9312204\RMSD=2.413e-09\RMSF=3.178e-06\Dipole=3.3100444,-1.107
 7991,4.5412911\Quadrupole=14.4015972,-8.5026501,-5.8989471,-22.3016348
 ,-1.2607309,-11.6898681\PG=C01 [X(C55H40N1O4P1)]\@

1-Naph/5 Type II E

1\1\GINC-WORKER0\FOpt\RTPSSTPSS\def2SVP\C55H40N1O4P1\JHIOE\19-Jan-2018

\0\#p tpsstps/def2svp int=ultrafine empiricaldispersion=gd3 opt scrf

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.6731045238\O,-1.2570521573,0.506124026,-2.1003712309\O,0.5466699911,0
 .8606358327,-0.3161322455\O,1.1832350304,0.1643449568,-2.8000123361\O,
 0.0622761123,-1.4999216823,-1.0312582867\C,-2.09750255,1.758912847,-0.
 247430118\C,-2.1980030983,0.6556227044,-1.1004770503\C,-3.2351651025,-
 0.3234910847,-0.987157681\C,-4.1893747233,-0.1487569374,0.00833073\H,-
 5.0056852774,-0.8725256348,0.1053462434\C,-4.1214705649,0.932088056,0.
 931211516\C,-3.0459250998,1.8884036612,0.8296341243\C,-2.9337504518,2.
 885714135,1.8455908421\H,-2.0979238857,3.5901802924,1.8129125228\C,-3.
 8553349531,2.9612721621,2.879863067\H,-3.7415954174,3.7301640705,3.651
 9199889\C,-4.9415273454,2.0475956514,2.9500865261\H,-5.6668496021,2.12
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 36296663,0.3233920586,2.0513490993\C,-0.9649744527,2.714567163,-0.4239
 614351\C,0.3449161016,2.2202534761,-0.4123986704\C,1.4947287681,3.0720
 136317,-0.4567742778\C,1.2877600057,4.439881688,-0.5954454422\H,2.1511
 05826,5.1135912422,-0.6264730237\C,-0.019499748,4.9950189122,-0.701599
 3608\C,-1.1689625093,4.1266098978,-0.6225750886\C,-2.4649663947,4.7045
 90755,-0.7827131942\H,-3.3444203446,4.0544373832,-0.7634212001\C,-2.62
 03734557,6.0693362091,-0.9754412725\H,-3.6246457017,6.4885896715,-1.10
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 0040474771,-1.1664235335\C,-0.214877534,6.3969183076,-0.889416959\H,0.
 6668308637,7.0460860749,-0.9376941672\C,5.2041394427,-2.3990153563,-1.
 4367728219\C,5.2719685672,-3.3641266419,-0.4080707179\H,6.0969858737,-
 4.0851236983,-0.4012614378\C,4.3031727565,-3.4233321942,0.5979454528\H
 ,4.3763759735,-4.1959935025,1.3692200689\C,3.2188172011,-2.5137779001,
 0.5971794151\C,3.1659365601,-1.5287918993,-0.4168036143\H,2.4045023599
 ,-0.7499586563,-0.3753652815\C,4.1310961941,-1.4819979168,-1.419213091
 8\H,4.0562930452,-0.7037559171,-2.1849229609\C,2.1883760418,-2.5721175
 129,1.6424158174\C,2.5390021995,-3.0914849567,3.0044000177\H,1.8825668
 553,-2.6647130886,3.7781232515\H,3.5879778653,-2.8577367262,3.23726094
 58\H,2.4232845555,-4.1906056965,3.0292818888\N,0.9795556564,-2.1359359
 374,1.3591460672\H,0.7318345734,-1.8279032705,0.3509442806\C,-0.147734
 5166,-2.0451770658,2.2360607045\C,-0.8416114092,-0.8209179903,2.264438
 8386\H,-0.4964486787,0.0072330227,1.6394545744\C,-1.9627787188,-0.6887
 723696,3.0927277341\H,-2.4911921657,0.2679568612,3.134495762\C,-2.4110
 780574,-1.7771679039,3.8587425302\C,-1.7328796746,-3.0045573987,3.7967
 404909\H,-2.0908724641,-3.8630577098,4.3745442707\C,-0.5976314893,-3.1
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 .2954354508,-1.6699362768,4.495612284\C,6.2597591848,-2.3145900151,-2.

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1-Naph/5 Type I Z

1\\1\\GINC-WORKER0\FOpt\RTPSSSTPSS\def2SVP\C55H40N1O4P1\\JHIOE\\24-Jan-2018
 \0\\#p tpsstps/def2svp empiricaldispersion=gd3 int=ultrafine opt scrf
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2789\H,-2.8654302311,1.788504963,0.3840435305\C,-4.2445193823,1.260728
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97464,1.5239988717,1.6917975321\C,0.6121323296,0.5963446559,2.12278914
94\H,1.4580092914,0.6352353026,1.4209553591\H,0.2372237344,-0.43392439
44,2.2136837151\H,0.9688679163,0.9116522396,3.1222116353\N,-0.18077747
23,2.4133416786,0.7710080859\H,0.7112082368,2.2064527644,0.2003404438\N
C,-0.9320560819,3.5323432536,0.3040669941\C,-0.9033642241,3.8164591207
,-1.074023423\H,-0.3422121815,3.1708181665,-1.7550858562\C,-1.61260852
63,4.922702151,-1.5610772547\H,-1.6014684182,5.1366491956,-2.634834859
4\C,-2.3308815785,5.7480962481,-0.6826573155\C,-2.3271256048,5.4736192
886,0.6959443458\H,-2.866699012,6.1278392871,1.3888661636\C,-1.6267026
57,4.370962376,1.1969241818\H,-1.61105533,4.161318113,2.2700167938\H,-
2.8832512154,6.6114551476,-1.0682504879\C,-5.8096618311,0.5619697224,3
.8178717383\H,-6.1660343962,-0.4081835583,3.4206469352\H,-5.8244039342
,0.5031967925,4.9186805878\H,-6.5357087132,1.3270372772,3.4910321551\C
,4.7337675215,-0.0055380014,-0.5198363396\C,5.123736248,1.2294666621,0
.1123480066\C,5.2919307388,-0.3497080785,-1.7501720271\C,4.5427409699,
1.6982033797,1.3306311324\C,6.1198509805,2.056683906,-0.5304785752\C,6
.2632446057,0.4694108561,-2.3784030957\H,4.9798748418,-1.2806217331,-2
.2342649759\C,4.9393997369,2.8982588527,1.9002789662\H,3.7583153908,1.
105078949,1.8085484455\C,6.5124408094,3.282464003,0.0892260118\C,6.678
4403603,1.6459824924,-1.7767835802\H,6.6861201947,0.1595086566,-3.3402
9188\C,5.9404942235,3.6953276733,1.281230845\H,4.4729347829,3.24001656
87,2.8310574723\H,7.2737923254,3.8966295742,-0.4054058743\H,7.43339146
72,2.2823145745,-2.2523730134\H,6.2488080408,4.6400233302,1.7426789906
\C,-2.7131662191,-0.4415595184,-1.983787312\C,-4.0345265129,-0.4466850
732,-1.3965693871\C,-2.3255045733,0.6340954445,-2.7822675584\C,-4.4904
138785,-1.4557741702,-0.4919950351\C,-4.9382965447,0.6401466233,-1.705
3787615\C,-3.210061619,1.7082862564,-3.0541763112\H,-1.3175089204,0.64
78222136,-3.21003796\C,-5.7747390938,-1.4301071978,0.0311904928\H,-3.8
077648175,-2.2574946084,-0.1969234404\C,-6.2573077483,0.6310260476,-1.
1559054355\C,-4.4948757274,1.7098094351,-2.5376345726\H,-2.8678474142,
2.5339438913,-3.6874365653\C,-6.6755881317,-0.3878944138,-0.3155623007
\H,-6.0939197462,-2.2146788487,0.7261395124\H,-6.9326825665,1.45615216
6,-1.4096426879\H,-5.186843775,2.5309511218,-2.7565605779\H,-7.6891492
96,-0.3812295354,0.0999849329\\Version=ES64L-G09RevD.01\\State=1-A\\HF=-
2815.9255238\\RMSD=7.578e-09\\RMSF=3.157e-06\\Dipole=-3.417377,0.9197017,
5.0585879\\Quadrupole=6.3354741,4.8617084,-11.1971824,-7.8389257,-3.408
6945,1.5981911\\PG=C01 [X(C55H40N1O4P1)]\\@

1-Naph/5 Type II Z

1\\1\\GINC-LOGI\\FOpt\\RTPSSTPSS\\def2SVP\\C55H40N1O4P1\\JHIOE\\23-Jan-2018\\
\\#p tpsstps/def2svp empiricaldispersion=gd3 int=ultrafine opt scrf=(
smd,solvent=ch2cl2,read)\\title\\0,1\\P,-1.0366091563,-0.0808495057,-2.
1650678362\\O,-2.2132591371,1.0718589996,-1.8434729753\\O,0.1287472111,0
.4156527835,-1.0279915429\\O,-0.5922705016,0.1354505243,-3.5811321101\\O
,-1.4722221864,-1.4394415212,-1.6175584402\\C,-1.7213238106,2.087329092
,0.2617211557\\C,-2.554786801,1.2835697322,-0.5216407688\\C,-3.738870448
2,0.6624499805,-0.0153144089\\C,-4.0890895073,0.9072404137,1.3065153116
\\H,-4.9984605266,0.4543999614,1.7159945345\\C,-3.272740708,1.6975708901
,2.1637298807\\C,-2.0493638104,2.2695109716,1.6551273835\\C,-1.186946937
,2.9368082008,2.5772045128\\H,-0.2294417704,3.3297541367,2.2252071482\\C
,-1.5356586186,3.0774473295,3.9124428939\\H,-0.8518468456,3.58738083,4.
599827412\\C,-2.7659604804,2.5592044732,4.3985836707\\H,-3.0325673688,2.
6839057632,5.4536597014\\C,-3.6124001019,1.8772959188,3.5392168957\\H,-4
.5505355933,1.4456595749,3.9059270466\\C,-0.464957823,2.6342503151,-0.3

279138033\C,0.4554464069,1.7494306075,-0.9077205676\C,1.773176572,2.15
81090127,-1.2923904498\C,2.100228157,3.5047386855,-1.1777865177\H,3.1
029741713,3.8402795407,-1.4635479463\C,1.1610728878,4.470709798,-0.719
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2,-0.9190524,6.426651\\PG=C01 [X(C55H40N1O4P1)]\\@

1-Naph/6 Type I E

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\H,0,-3.920693,1.768452,1.579474\C,0,-5.155567,0.20229,2.380557\H,0,-5
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\C,0,4.24226,-0.339842,-0.451442\C,0,4.014197,0.818195,-1.218757\H,0,3
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\C,0,-1.829728,-2.6908,-3.68506\C,0,-0.500346,-3.921159,-0.378488\C,0,
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1-Naph/6 Type II E

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1-Naph/6 Type I Z

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 \O,-1.7415376372,-1.6595243541,-0.9372063561\C,-1.608678336,2.11754555
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 .9408962835,-0.6021766297\H,-1.8201192124,4.7542613051,-0.1404980004\C
 ,-0.4485102189,6.2424097082,-0.8706603225\H,-1.1110920025,7.0761351556
 ,-0.6132822788\C,0.8061881564,6.5042525666,-1.4847361894\H,1.108727605
 3,7.5371417556,-1.6886950336\C,1.6362788476,5.4513130892,-1.8341100924
 \H,2.6008121498,5.6377683354,-2.3200078601\C,4.3861429653,-1.039486241
 6,3.3827201567\C,3.2131302014,-0.9214048536,4.1670021046\H,3.313421772
 5,-0.6689092851,5.2269221622\C,1.9641133114,-1.1132121824,3.589270621\
 H,1.0694283269,-1.012531828,4.2106440619\C,1.8419512081,-1.4716384109,
 2.2206595585\C,3.02403554,-1.5742276353,1.4453944938\H,2.9612167063,-1
 .7856882866,0.3748409395\C,4.2797472603,-1.3535413016,2.0070009367\H,5
 .1646051309,-1.4049183947,1.368730151\C,0.5219230525,-1.610530743,1.60
 77736136\C,-0.6164645239,-0.7620594072,2.0916915567\H,-1.4414947401,-0
 .7671845877,1.3643911133\H,-0.2833803187,0.2692965668,2.2813270502\H,-
 0.9880442888,-1.1769190912,3.0482501212\N,0.2604133414,-2.4267023027,0
 .6051706586\H,-0.6350068247,-2.2075845037,0.0506377585\C,1.0422988246,
 -3.490949409,0.0669992622\C,1.0602404445,-3.6594335716,-1.3299581575\H
 ,0.5140018076,-2.9646619672,-1.9737296222\C,1.7945725657,-4.7165495426
 ,-1.8853739933\H,1.8179295726,-4.83976484,-2.9730796624\C,2.4946084022
 ,-5.6069065946,-1.0575061606\C,2.4460466096,-5.4479646801,0.3385011418
 \H,2.9710180021,-6.1535091864,0.9912328517\C,1.7185607143,-4.397015602
 7,0.9072234787\H,1.6677116723,-4.2781037413,1.9931273557\H,3.067415767
 8,-6.4307010146,-1.4962077956\C,-4.7457682515,-0.0179463704,-0.4651663
 868\C,-5.1250183016,-1.2847472757,0.1078156184\C,-5.3208567268,0.38684
 56285,-1.6690533501\C,-4.5280318709,-1.8130730362,1.2935687998\C,-6.12
 80717861,-2.0809755958,-0.5629224764\C,-6.2978457479,-0.4024275486,-2.
 3259433682\H,-5.017887884,1.3423526759,-2.1088922902\C,-4.9163848776,-

3.0404172461,1.8079846814\H,-3.7382943572,-1.2434780809,1.790638465\C,
-6.512125194,-3.3364935305,0.0002813103\C,-6.7028149938,-1.6092944957,
-1.7797966203\H,-6.733856689,-0.0452303316,-3.2653061942\C,-5.92491408
44,-3.8070084419,1.1631590269\H,-4.43748028,-3.4270083052,2.7145814163
\H,-7.2793167452,-3.9264466147,-0.5144212778\H,-7.4623835228,-2.222378
914,-2.277907709\H,-6.2266299487,-4.7736597552,1.5814763054\C,2.648940
6122,0.5691834486,-2.0825583158\C,3.9715958851,0.5039465521,-1.5045232
183\C,2.2470269299,-0.4165096081,-2.982958017\C,4.4459544189,1.4276293
89,-0.521703172\C,4.8585492408,-0.5635085817,-1.9136685339\C,3.1185487
743,-1.4685787145,-3.3624503429\H,1.2349086368,-0.3811305494,-3.399337
7899\C,5.7331559523,1.3417864997,-0.0131599806\H,3.7759729671,2.212135
4363,-0.1588721942\C,6.17798769,-0.6228298207,-1.3687917811\C,4.401716
2047,-1.5401077153,-2.8468412525\H,2.7661248615,-2.2226556272,-4.07451
45045\C,6.6154374839,0.3171581456,-0.4500230072\H,6.069036423,2.063817
3519,0.739136785\H,6.8414048325,-1.4314684658,-1.6965705157\H,5.082085
0522,-2.3461599341,-3.1441656399\H,7.6323865966,0.2629884816,-0.046645
0056\O,5.5510103237,-0.8247770415,4.0275127424\C,6.7837687907,-0.90904
13031,3.2933555454\H,6.8138840365,-0.154847914,2.487363912\H,7.5789071
355,-0.7026375394,4.0243326964\H,6.9240957865,-1.9187974499,2.86698182
62\\Version=ES64L-G09RevD.01\State=1-A\HF=-2891.0904002\RMSD=3.489e-09
\RMSF=3.236e-06\Dipole=4.3031593,-1.1988808,4.7424329\Quadrupole=17.17
15427,1.6208173,-18.79236,-10.2848872,0.6543408,-1.0114541\PG=C01 [X(C
55H40N1O5P1)]\@

1-Naph/6 Type II Z

1\1\GINC-WORKER0\FOpt\RTPSSTPSS\def2SVP\C55H40N1O5P1\JHIOE\30-Jan-2018
\O\#p tpsstps\def2svp empiricdispersion=gd3 int=ultrafine opt scrf
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.148704571\O,-2.2499091233,0.9959200695,-1.8088768712\O,0.1053386841,0
.3685997815,-1.0037485607\O,-0.6109727974,0.1204492917,-3.5605006055\O
,-1.4651901324,-1.5052483009,-1.6265571028\C,-1.784479649,1.9662013592
,0.322542736\C,-2.6009146161,1.1679828328,-0.4841142762\C,-3.775899431
2,0.5133252648,0.0015509981\C,-4.1337019197,0.7170934568,1.3283506143\H,
-5.0368879769,0.2390334598,1.7225904997\C,-3.3345382306,1.4998119747
,2.2083853651\C,-2.1206807851,2.1073749795,1.7188150198\C,-1.275256412
9,2.7694678892,2.6601021222\H,-0.3246294979,3.1897695312,2.3212856181\H,
-1.6319895225,2.8719131864,3.9966910257\H,-0.9611533593,3.3788916244
,4.6988814175\C,-2.8537361935,2.3183585379,4.4650736307\H,-3.126963302
,2.4130016956,5.5215808118\C,-3.6831082358,1.640237663,3.5862344346\H,
-4.6141941016,1.1820266115,3.9383813239\C,-0.5382624668,2.5543481176,-
0.2496046906\C,0.4033197288,1.7050922935,-0.8494591093\C,1.7133873732,
2.1545481066,-1.219451068\C,2.0069842704,3.505702002,-1.0685952143\H,3
.0013661012,3.8724426126,-1.3452915901\C,1.0451083827,4.4376818517,-0.
5883319482\C,-0.2520563142,3.9637769667,-0.1733821682\C,-1.2111743551,
4.92325114,0.2722776579\H,-2.2109759996,4.5837943406,0.5587436516\C,-0
.8973974426,6.2730031089,0.3315831702\H,-1.6524307384,6.991276827,0.66
97037175\C,0.391723609,6.7339907883,-0.0500222641\H,0.627804714,7.8021
830811,0.0064925961\C,1.340222362,5.8322689639,-0.505133054\H,2.33315
0049,6.1758105026,-0.8168471553\C,5.3328876849,-2.718525674,1.27254946
38\C,5.0519164081,-3.6530537308,0.2500846019\H,5.8208221705,-4.3379105
859,-0.1146086514\C,3.7752274329,-3.6939308248,-0.313305284\H,3.578341
1437,-4.4183963031,-1.1090210157\C,2.7402403018,-2.8407153159,0.138416
4017\C,3.0437477765,-1.9058959568,1.1681825752\H,2.2892053771,-1.18750
01306,1.4981754234\C,4.313141511,-1.8432716744,1.7206628809\H,4.557468
4724,-1.1019478352,2.4860682846\C,1.4439889403,-2.8226776705,-0.536761
8498\C,1.3601253958,-3.1492474272,-1.998189638\H,0.3591332503,-2.92665

96867,-2.3956465957\H,1.5617645162,-4.2284801061,-2.1334319898\H,2.127
0493347,-2.5951433576,-2.5619282891\N,0.3167258923,-2.4803424837,0.056
2187548\H,-0.4858197832,-2.1865380111,-0.6004050726\C,0.043664254,-2.3
47739796,1.4504013874\C,-0.6685653468,-1.2183857138,1.8901186818\H,-0.
956510258,-0.4489530672,1.1693894684\C,-0.9814488652,-1.0909261239,3.2
502972269\H,-1.5262650631,-0.2062178106,3.5942155867\C,-0.5995257877,-
2.0878481618,4.1614488114\C,0.0947079445,-3.2230011897,3.7084179743\H,
0.3810445944,-4.0110643615,4.4129746507\C,0.4177190342,-3.3610560206,2
.353149715\H,0.9495315793,-4.2458031395,1.9902750319\H,-0.8487408271,-
1.9849484242,5.2228794363\C,-4.5664511272,-0.3824363148,-0.89258077\C,
-4.673196008,-1.7897074038,-0.6037619314\C,-5.2027229005,0.1364403571,
-2.0177287585\C,-3.9818042107,-2.4111658075,0.4805982289\C,-5.47613438
97,-2.6217522115,-1.4698204801\C,-5.9865885516,-0.686167222,-2.8667663
009\H,-5.1013382242,1.2024650764,-2.2451833021\C,-4.0930181822,-3.7722
358398,0.7169992044\H,-3.3372482781,-1.8021132511,1.1194013652\C,-5.58
09288112,-4.0189111426,-1.189306466\C,-6.129959488,-2.0369533089,-2.59
45594319\H,-6.4814177963,-0.2419914722,-3.7374555002\C,-4.9078740747,-
4.5844474851,-0.118431422\H,-3.5417635675,-4.2256805849,1.5485845945\H
,-6.1993669736,-4.6395098328,-1.8481256125\H,-6.7380753377,-2.67676542
59,-3.2441370707\H,-4.9929592831,-5.6584527703,0.0811554644\C,2.749218
7081,1.1978639088,-1.7150358186\C,3.9886396211,1.0218351258,-0.9949827
058\C,2.5353384536,0.4856489692,-2.8940505828\C,4.2617518593,1.6516986
056,0.2586813553\C,4.9957584957,0.1406908927,-1.5440806147\C,3.5274302
27,-0.3811132791,-3.4203459583\H,1.5791356116,0.5900095309,-3.41736284
38\C,5.4675605855,1.4549358165,0.9158575751\H,3.4993276715,2.292459749
2,0.7112306416\C,6.2266214049,-0.0363987216,-0.8420013467\C,4.73723466
2,-0.5463465514,-2.7664700118\H,3.3274378413,-0.9151206221,-4.35591560
86\C,6.4651913742,0.6113081225,0.3586736705\H,5.6474225006,1.945932860
1,1.8786882709\H,6.9790442491,-0.7078667882,-1.2712580055\H,5.50845631
81,-1.2109663393,-3.1720596251\H,7.4093872815,0.4563088175,0.891205494
6\O,6.5342736346,-2.5705970269,1.8665582462\C,7.6352583776,-3.38984663
46,1.4416607229\H,8.4904463092,-3.0790675645,2.0591267668\H,7.42361513
48,-4.4606709557,1.6138342937\H,7.8670007772,-3.2177661818,0.374841040
9\Version=ES64L-G09RevD.01\State=1-A\HF=-2891.0941039\RMSD=5.614e-09\
RMSF=1.710e-06\Dipole=4.69383,-3.3567795,3.8048099\Quadrupole=18.68447
48,9.1563957,-27.8408705,-26.4593865,-5.3008169,7.8861974\PG=C01 [X(C5
5H40N1O5P1)]\@

1-Naph/7 Type I E

1\1\GINC-WORKER1\FOpt\RTPSSTPSS\def2SVP\C55H37F3N1O4P1\JHIOE\19-Jan-20
18\0\#p tpsstps\def2svp empirical dispersion=gd3 opt int=ultrafine sc
rf=(smd,solvent=ch2cl2,read)\title\0,1\P,0.3145670587,0.2773436145,-
1.6714639833\O,-1.227856796,-0.1959820501,-2.1349313104\O,-0.114513485
4,1.1387283021,-0.273265518\O,0.8494646491,1.1805697402,-2.7416082643\
O,1.0766805998,-0.9195925281,-1.1072681259\C,-2.7442907911,0.238830143
5,-0.3329022531\C,-2.093222582,-0.6751150626,-1.1697358862\C,-2.290399
8228,-2.0905780138,-1.0795089072\C,-3.1931112659,-2.5630852083,-0.1340
244386\H,-3.3800075058,-3.6392638251,-0.055677916\C,-3.8670857403,-1.6
879867226,0.7635413816\C,-3.6199934978,-0.2679056888,0.6946230468\C,-4
.2163682274,0.5655230564,1.6894574518\H,-4.0029334384,1.6378458626,1.6
874695427\C,-5.0476388143,0.0345573723,2.6649785977\H,-5.4873792264,0.
6956862112,3.4198547851\C,-5.3268661164,-1.3577220214,2.6997803672\H,-
5.9851738391,-1.7637136064,3.4753828799\C,-4.7406152177,-2.2000472444,
1.7699278264\H,-4.9156203083,-3.2807857729,1.8075818276\C,-2.434184320
7,1.6933158177,-0.4604504618\C,-1.0978985638,2.098085482,-0.3788312699
\C,-0.6934338635,3.4703312049,-0.3773372822\C,-1.6784968689,4.43884673

08,-0.5234262512\H,-1.3992752038,5.4981244153,-0.5193880456\C,-3.05055
72914,4.0896694049,-0.6883203248\C,-3.4425928965,2.700142262,-0.672269
1397\C,-4.815427025,2.3819322263,-0.9012912399\H,-5.1210502835,1.33178
89924,-0.9294211846\C,-5.757612921,3.3804902457,-1.0999334264\H,-6.804
4193614,3.1113664948,-1.2789095656\C,-5.375934392,4.7489460044,-1.0795
046132\H,-6.1308033088,5.5280989237,-1.2315256643\C,-4.0477809527,5.09
2561345,-0.8837839902\H,-3.7378291575,6.1437975755,-0.8839573936\C,-0.
3621459504,-2.5942376618,3.4635590121\C,0.8916955378,-3.127956616,3.80
27180513\H,0.9629207383,-3.9659854893,4.5012652165\C,2.0506986669,-2.5
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598887452,-1.5247651423,2.3104034511\C,0.6939063855,-0.9867940395,1.98
78651925\H,0.6045064021,-0.142585639,1.3014697316\C,-0.4602084652,-1.5
140947351,2.5700631841\H,-1.4366443847,-1.0897282854,2.319042235\C,3.1
971481535,-0.9831110883,1.7033157973\C,4.4275315936,-0.8624033839,2.54
87583048\H,5.1037987581,-0.0816214529,2.1688251735\H,4.9776667233,-1.8
216474252,2.5536744413\H,4.140819136,-0.6396703523,3.5876067594\N,3.15
95199845,-0.613393542,0.4467608661\H,2.2365144851,-0.7380117125,-0.125
8361939\C,4.2258511029,-0.093103085,-0.3521292814\C,3.9336754144,0.997
9008494,-1.1929306496\H,2.9352583688,1.4416757487,-1.2013577863\C,4.93
95352041,1.5172889502,-2.0166691776\H,4.7129707143,2.3741443569,-2.659
0883695\C,6.2217650183,0.9458013391,-2.0192575444\C,6.4956633268,-0.16
13638081,-1.2005514868\H,7.4865342328,-0.6271249284,-1.2154975644\C,5.
5011249841,-0.6897282375,-0.3672599148\H,5.7055127621,-1.5754663537,0.
2391788239\H,7.0035295413,1.3538202249,-2.668577209\C,-1.6253745626,-3
.2139117123,4.0068118821\C,-1.531847884,-3.0105273445,-1.976494933\C,-
0.6514110423,-4.0153827958,-1.4345615268\C,-1.6598466636,-2.8887553817
,-3.3590936677\C,-0.4158943509,-4.1704426783,-0.034266246\C,0.05565722
31,-4.8880124426,-2.3448579518\C,-0.9658299018,-3.7497035468,-4.246123
9987\H,-2.3159404214,-2.1136708558,-3.7671061463\C,0.4493389667,-5.140
7684176,0.4468160786\H,-0.9204691849,-3.5053871637,0.6695036597\C,0.93
6848352,-5.8798779478,-1.8152315071\C,-0.1274390271,-4.7348854818,-3.7
507723445\H,-1.100913944,-3.6297452415,-5.3266608688\C,1.1302024473,-6
.008671336,-0.4493986525\H,0.6104407857,-5.2335204669,1.5264334737\H,1
.4642026799,-6.5369635238,-2.5164871337\H,0.4113050351,-5.4054079308,-
4.4299553563\H,1.8108948476,-6.7730125436,-0.0582831215\C,0.7534156227
,3.8198967664,-0.2744769611\C,1.54559744,3.4271238126,0.8641543158\C,1
.357375598,4.5179382031,-1.3182762858\C,0.9928098031,2.7559513147,1.99
63173242\C,2.9573509095,3.7309760575,0.8719534227\C,2.7409973226,4.832
4345155,-1.2951500553\H,0.754794647,4.7978756482,-2.1886668037\C,1.791
2696175,2.3667002366,3.0608045296\H,-0.0801357867,2.5426512354,2.01897
94916\C,3.753737668,3.3091510155,1.9799322975\C,3.5294171396,4.4375798
565,-0.2274382353\H,3.1835524014,5.3722198318,-2.1393624028\C,3.186940
4921,2.6360434668,3.0504739425\H,1.3445999236,1.8450075284,3.914176325
9\H,4.8269883516,3.5307807846,1.9671802516\H,4.6033107499,4.6547881781
,-0.2144696434\H,3.8099636855,2.3147501245,3.892223607\F,-2.5439939389
,-2.278440618,4.3546434077\F,-1.4032679388,-3.9846660647,5.0981522235\F
,-2.2216696734,-4.0172489215,3.0774292231\\Version=ES64L-G09RevD.01\State=1-A\HF=-3113.4497871\RMSD=3.338e-09\RMSF=3.177e-06\Dipole=4.43544
1,-0.7479452,3.7612463\Quadrupole=33.1028976,-10.980024,-22.1228736,-1
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1-Naph/7 Type II E

1\1\GINC-WORKER0\FOpt\RTPSSTPSS\def2SVP\C55H37F3N1O4P1\JHIOE\19-Jan-20
18\0\#p tpsstps\def2svp empiricaldispersion=gd3 opt int=ultrafine sc
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-1.659648646\O,-1.2742214023,0.4440017592,-2.0796032856\O,0.524357656,

0.8546057897,-0.3016073259\O,1.1724780355,0.1795916134,-2.7896837344\O
,0.1141770224,-1.5181239707,-1.0167593676\C,-2.1530144154,1.6586892232
, -0.217195236\C,-2.2198032758,0.5592054368,-1.0783866354\C,-3.23027571
44,-0.4484264017,-0.978145481\C,-4.1930086305,-0.3092305735,0.01419462
66\H,-4.9893167473,-1.0561310249,0.1018895372\C,-4.1567272871,0.764155
3323,0.9478905042\C,-3.1065239794,1.7496145009,0.8597747429\C,-3.02351
6338,2.7386992557,1.88640401\H,-2.2058530821,3.4643478517,1.8640161479
\C,-3.9507534929,2.7798499641,2.9175276415\H,-3.8593820586,3.542526357
2,3.6985925319\C,-5.0126329174,1.8372060025,2.9746215677\H,-5.74188883
9,1.8855614661,3.790526921\C,-5.1089423411,0.8486406716,2.0084235719\H
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25184,-1.5053114012\H,3.2372518004,3.4174123556,-2.3341236315\C,3.0279
691177,0.7660151682,2.9065369241\H,1.4799493715,1.8810477674,1.9184276
087\C,5.1745921809,0.6071222933,1.7775774842\C,5.4881264294,1.67541167
27,-0.445394722\H,5.6020733806,2.6218204283,-2.3787760746\C,4.37036922
21,0.3001802297,2.8630140616\H,2.3965011247,0.5253366067,3.7688556054\

H,6.2111681686,0.2540516043,1.7347785919\H,6.5159094621,1.2978329893,-
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-0.8577460414,-2.406125035\F,7.120301186,-3.0208893495,-2.6378580359\F
,5.6695957615,-1.9035098982,-3.8272258613\\Version=ES64L-G09RevD.01\St
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049288,6.4833139,-20.6276541\PG=C01 [X(C55H37F3N1O4P1)]\@

1-Naph/7 Type I Z

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1-Naph/7 Type II Z

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9-Phen/5 Type I E

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9-Phen/5 Type I Z

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2.6920729594,0.5855228645,-2.0393047913\C,3.994616018,0.481761259,-1.3945145691\C,2.3060342587,-0.3720452305,-2.9511869795\C,4.4037097583,1.3953401251,-0.3817313723\C,4.887843723,-0.5871575025,-1.7614726807\C,3.1540234616,-1.4697207616,-3.3148041078\H,1.3149332054,-0.3125668699,-3.4130968573\C,5.6566711359,1.3077141591,0.2138397092\H,3.7106605526,2.1788001169,-0.0628902062\C,6.1662746964,-0.6404811333,-1.140599863\C,4.4594867657,-1.5900435426,-2.7337972669\C,6.5531882254,0.2905707801,-0.1821575985\H,5.9430633874,2.0224573921,0.9929537829\H,6.8661618655,-1.4346094535,-1.415052741\H,7.5446583684,0.2199987409,0.2780934759\C,2.7046083067,-2.442603627,-4.251501189\C,3.5158195048,-3.510993354,-4.6129404066\C,5.2645854779,-2.6950517344,-3.123641917\C,4.8045620404,-3.635657452,-4.0414671891\H,5.4461463345,-4.478684805,-4.3205240214\H,3.1590712277,-4.2575656923,-5.3308130324\H,6.2638833933,-2.8216576193,-2.6975964437\H,1.6995110558,-2.3358835714,-4.6740427242\C,-6.8055196645,-0.1557979785,-3.6107311998\C,-7.7630301781,-0.9502156333,-4.2290195357\C,-7.6261255331,-2.5507919281,-2.3966601473\C,-8.1752110092,-2.1559593048,-3.6136531361\H,-6.4765713873,0.7816671532,-4.073328998\H,-8.1978561711,-0.6465334248,-5.1875373788\H,-8.9303720209,-2.7852348155,-4.0973865833\H,-7.9622856891,-3.4898854721,-1.9478849536\\Version=ES64L-G09RevD.01\\State=1-A\\HF=-3123.086959\\RMSD=4.644e-09\\RMSF=3.516e-06\\Dipole=3.4752457,-1.2236716,5.1112733\\Quadrupole=4.8824302,1.6554085,-6.5378387,-7.7577928,11.3044554,0.8065922\\PG=C01 [X(C63H44N1O4P1)]\\@

9-Phen/5 Type II Z

1\\GINC-LOGIN\FOpt\RTPSSTPSS\def2SVP\C63H44N1O4P1\JHIOE\13-Apr-2018\O\\#p tpsstps/def2svp empiricaldispersion=gd3 int=ultrafine opt scrf=(smd,solvent=ch2cl2,read)\\title\\0,1P,-1.0254040774,-0.1252489562,-2.1311024411\O,-2.244556207,0.9830445234,-1.8136382315\O,0.1170715197,0.4138450695,-0.9891897003\O,-0.5823596567,0.1067748869,-3.5459304242\O,-1.4196253896,-1.4973583942,-1.5870543031\C,-1.8136365374,1.9752710054,0.3136699916\C,-2.6079796698,1.1541518568,-0.4913163043\C,-3.7698789304,0.4758354362,-0.0063835062\C,-4.13619695,0.6795134456,1.318533675\H,-5.0308505011,0.1858130306,1.7128663808\C,-3.3566356743,1.4832620266,2.1970996874\C,-2.1561848049,2.1167083916,1.7073945537\C,-1.3283343667,2.8045307716,2.6456645076\H,-0.3878274224,3.2454631749,2.3047882907\C,-1.6896062106,2.9051543257,3.9810643385\H,-1.0329093015,3.4325076801,4.6815586351\C,-2.8978894804,2.323208366,4.4504499812\H,-3.17443049,2.4168967725,5.506209891\C,-3.709923886,1.6212995843,3.5740915487\H,-4.6300518798,1.1427659629,3.9279308012\C,-0.5816941983,2.590657891,-0.259587824\C,0.3825042642,1.759493102,-0.8476347241\C,1.6801236972,2.2403725039,-1.2226939764\C,1.9338078768,3.602178449,-1.097075173\H,2.9163075642,3.9936437796,-1.3821500963\C,0.9451440881,4.5131710834,-0.6310839797\C,-0.3353620966,4.007925705,-0.2015299168\C,-1.3205621977,4.9448695642,0.235352766\H,-2.3077508468,4.5803259737,0.5346694719\C,-1.0465221042,6.3039583329,0.2721340547\H,-1.8206035799,7.004584271,0.6041926064\C,0.2257419774,6.7971294241,-0.1256428828\H,0.4299896626,7.8726816191,-0.0868080707\C,1.1985904109,5.9171690144,-0.5719959242\H,2.1789467015,6.2855059805,-0.8950455256\C,5.4183281368,-2.8464888221,1.2122510979\C,5.0484122397,-3.8196575022,0.2619909489\H,5.7790608683,-4.5742048472,-0.0493502762\C,3.7676235897,-3.8330925564,-0.2997739189\H,3.5127442056,-4.5981277885,-1.0388784911\C,2.8016259019,-2.8827741303,0.0995228593\C,3.1713736791,-1.894269365,1.0470797509\H,2.4608731036,-1.1117553114,1.3274168272\C,4.4569210829,-1.8783876518,1.5835066953\H,4.7312420622,-1.0900231462,2.2921181408\C,1.4847938343,-2.8341236562,-0.554149241\C,1.3706926406,-3.1726926265,-2.0081487811\H,0.3626084892,-2.9567863837,-2.3906630796\H,1.5778734905,-4.2519814261,-2.1345669844\H,2.127

5292678,-2.6259450814,-2.5927467497\N,0.3859934474,-2.458549866,0.0626
634424\H,-0.4320565345,-2.1652708032,-0.5807442511\C,0.1491855877,-2.2
951545301,1.4610404835\C,-0.5882788976,-1.1754590644,1.8846091387\H,-0
.9210197097,-0.4389012539,1.149215254\C,-0.8691076267,-1.014115731,3.2
480894431\H,-1.4340286018,-0.1370600879,3.5788358499\C,-0.4300260911,-
1.9676874682,4.1794575036\C,0.2864990329,-3.0952861567,3.7430460356\H,
0.6155874949,-3.8516935998,4.4633547853\C,0.5783800948,-3.2670243697,2
.3847962916\H,1.1237602539,-4.1495387263,2.0383477867\H,-0.6540042291,
-1.8379097937,5.2435267377\C,6.8008426023,-2.8154141941,1.8121760388\H
,6.7572838484,-3.0036122074,2.9013043676\H,7.4601247467,-3.572276406,1
.3569344821\H,7.2612203613,-1.8199405626,1.6771667253\C,-4.5407148529,
-0.4333349637,-0.9039002753\C,-4.6506825397,-1.8517545417,-0.601006387
\C,-5.1434338505,0.0713520969,-2.0344940066\C,-3.9586053935,-2.4311819
499,0.4993792842\C,-5.4344701614,-2.7039801549,-1.4544498721\C,-5.9258
379663,-0.7464348623,-2.9163210317\H,-5.0393279545,1.1348111092,-2.273
9470392\C,-4.0492804704,-3.7887761107,0.7803118249\H,-3.3264691524,-1.
7936125351,1.1221945946\C,-5.5170946908,-4.086886714,-1.1313687665\C,-
6.0970609042,-2.141703895,-2.6289559997\C,-4.845457928,-4.6225442134,-
0.0373999409\H,-3.4978415197,-4.2094668038,1.6284915813\H,-6.113539096
2,-4.7543998128,-1.759760217\H,-4.9265666168,-5.6932203413,0.180192634
8\C,2.7344977834,1.2976394629,-1.7032968282\C,3.990459753,1.1542356349
,-0.9788245857\C,2.5184818898,0.5577911906,-2.8449636269\C,4.232822659
1,1.8432072171,0.2440155317\C,5.0096896079,0.2715099187,-1.4859734095\
C,3.4980068454,-0.352904268,-3.3624050347\H,1.563588647,0.6446622021,-
3.374203714\C,5.4396387043,1.7187727862,0.9227657469\H,3.4475836119,2.
4815310718,0.6584094954\C,6.2352547226,0.1753360465,-0.7718985724\C,4.
7553785292,-0.5120759959,-2.6919095429\C,6.4567396545,0.8893917926,0.4
008902366\H,5.5977385733,2.2619323581,1.8607846613\H,7.0268460521,-0.4
808683265,-1.1433897613\H,7.4134928838,0.7937996573,0.9253078063\C,3.2
172923913,-1.1180472321,-4.5299204017\C,4.1449695647,-2.0251107272,-5.
0269771272\C,5.6827970771,-1.4482364668,-3.2255810307\C,5.3854377422,-
2.1897899486,-4.3658975944\H,6.1182019882,-2.9073371668,-4.7510330071\
H,2.2456617986,-0.9869819062,-5.0186541358\H,6.647488731,-1.6048913291
,-2.7348857141\H,3.9179806992,-2.6139559048,-5.9223685957\C,-6.5455193
498,-0.1822422484,-4.0665622513\C,-6.8953284828,-2.9130588363,-3.51708
51907\C,-7.3177972059,-0.9638704239,-4.9169013625\C,-7.4935557519,-2.3
394665943,-4.6358385884\H,-6.4016360806,0.8852324075,-4.2688426695\H,-
7.7899388862,-0.5190786504,-5.7997146196\H,-8.1029621292,-2.9595334624
,-5.3024789577\H,-7.0484786413,-3.9793242441,-3.3283289602\\Version=ES
64L-G09RevD.01\State=1-A\HF=-3123.0907223\RMSD=5.477e-09\RMSF=3.818e-0
6\Dipole=3.865182,-2.8205872,4.0031764\Quadrupole=8.1044286,6.8363465,
-14.9407751,-16.8672175,6.0429655,7.834008\PG=C01 [X(C63H44N1O4P1)]\@

9-Phen/6 Type I E

1\1\GINC-LOGIN\FOpt\RTPSSTPSS\def2SVP\C63H44N1O5P1\JHIOE\10-Aug-2018\0
\\#p tpsstps\def2svp empiricaldispersion=gd3 int=ultrafine opt scrf=(
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275475356\O,-0.8128612885,0.4503797688,-2.2938220402\O,0.825361467,0.8
44030439,-0.3792299195\O,1.5438453061,-0.5168456597,-2.5425361609\O,-0
.086581692,-1.4824975509,-0.6568877188\C,-1.4040349778,2.3880604041,-1
.0113841922\C,-1.7419525055,1.1353910777,-1.5396644423\C,-3.0302555611
,0.5409700736,-1.3545389974\C,-3.992535269,1.2580706833,-0.6556363812\
H,-4.9918960224,0.8310934063,-0.5183730305\C,-3.7049629832,2.527863362
3,-0.079071645\C,-2.3813626971,3.0873473414,-0.2145320312\C,-2.0906264
646,4.2989956686,0.4849840747\H,-1.0789127722,4.7117242072,0.440892950
1\C,-3.0663365862,4.9529078326,1.223027599\H,-2.8156836515,5.879007995

3,1.7517836472\C,-4.3854817551,4.4305772477,1.303879455\H,-5.149113549
9,4.9618512398,1.8820799135\C,-4.6917995065,3.2365581895,0.6716964928\
H,-5.6956914158,2.8045883983,0.7512592653\C,-0.0247295191,2.9193242643
, -1.2151697428\C,1.0583219061,2.1213911008,-0.8340847171\C,2.414538712
,2.5731325131,-0.8690055185\C,2.6684533557,3.8403967116,-1.3754189341\
H,3.6975177476,4.2142280137,-1.4102852918\C,1.6165900252,4.6695604763,
-1.8652744391\C,0.2495162605,4.2096400903,-1.7964996316\C,-0.771559910
4,5.042788584,-2.345665264\H,-1.8079442597,4.6929949129,-2.3353732609\
C,-0.4670243723,6.2763762095,-2.9024933241\H,-1.2681214074,6.894538128
6,-3.322449213\C,0.8745641068,6.7417263238,-2.9389049982\H,1.101418541
5,7.7196940833,-3.3771991622\C,1.8935176791,5.9491039965,-2.4345928162
\H,2.9348763687,6.2885919282,-2.4727100931\C,-2.0426379904,0.246654315
,4.0603699106\C,-1.537245938,-0.7888124182,4.8853251308\H,-1.976249476
, -0.9298317857,5.8775126319\C,-0.5071580331,-1.6038557404,4.4342412027
\H,-0.143702087,-2.4004617223,5.0894432597\C,0.0417438183,-1.437340273
9,3.1321771673\C,-0.4687435514,-0.3900036993,2.325610275\H,-0.04684030
65,-0.1954035683,1.3387512914\C,-1.4874797734,0.4463948607,2.774646544
2\H,-1.8361197779,1.2525468376,2.1251564846\C,1.1288536243,-2.30023793
96,2.6727776527\C,1.9856489847,-3.0132622161,3.6791673548\H,2.98594943
3,-3.2258298469,3.2729697475\H,1.5202765455,-3.9758224067,3.9597087582
\H,2.0858407607,-2.4075741944,4.5911576698\N,1.3622411924,-2.422775977
9,1.3781784213\H,0.723767275,-1.9442699597,0.659643569\C,2.3957937559,
-3.1758070477,0.7355993006\C,3.1260497524,-2.5352548296,-0.2832124748\
H,2.9253488413,-1.4915174037,-0.5355507761\C,4.1268302262,-3.241387763
7,-0.9616239896\H,4.7037541148,-2.732383824,-1.7404372595\C,4.39341417
98,-4.5813618235,-0.639321389\C,3.642284312,-5.2220644561,0.3589355994
\H,3.8292802592,-6.2736206841,0.6010498338\C,2.6375618163,-4.527231339
2,1.0461766163\H,2.0291571864,-5.0365980454,1.7975591227\H,5.179003145
8,-5.1283147489,-1.1714370895\C,-3.3000146056,-0.824768779,-1.89867682
23\C,-3.4597699346,-1.9552411425,-0.9991402616\C,-3.364996521,-1.02068
4763,-3.2594091319\C,-3.3410662779,-1.8000015401,0.4098328367\C,-3.704
1420721,-3.2663028655,-1.5367534203\C,-3.614436717,-2.3109129417,-3.83
66437421\H,-3.2229972968,-0.17161995,-3.9365259088\C,-3.4705539808,-2.
8816586676,1.2719836558\H,-3.1244234001,-0.8090086607,0.8149928451\C,-
3.8354691836,-4.3518328464,-0.6270560193\C,-3.7928183469,-3.4506123615
, -2.9832254568\C,-3.7242609371,-4.1692719219,0.7475735894\H,-3.3668155
476,-2.7359572098,2.3528003694\H,-4.0222745746,-5.3588723998,-1.010444
9516\H,-3.8274361825,-5.027175941,1.4211267311\C,3.5013946871,1.662561
4377,-0.4040711089\C,3.552019408,1.1957714761,0.9728751532\C,4.4494394
609,1.2327000139,-1.3051069838\C,2.6111147041,1.6446485639,1.940765939
2\C,4.5723597773,0.2657677437,1.373854512\C,5.4868666313,0.3081501623,
-0.9436474512\H,4.3927345114,1.5668622855,-2.3464591403\C,2.6460037697
,1.1875126504,3.2522776303\H,1.8420206699,2.3624015546,1.6406753038\C,
4.5807097824,-0.1829320063,2.7233223198\C,5.5582206828,-0.1929663323,0
.3983030251\C,3.6385893272,0.2618452103,3.6452481871\H,1.9028712519,1.
5397248726,3.9754990889\H,5.3429151272,-0.8941745904,3.0531590086\H,3.
6712309342,-0.1042617115,4.6769086091\C,-4.0385211871,-4.7105456943,-3
.5939630293\C,-3.6878632564,-2.4701355078,-5.2489084749\C,-3.929772632
2,-3.7156112211,-5.8153803678\C,-4.1065483789,-4.8425778865,-4.9782362
964\H,-3.5473877649,-1.5880310199,-5.8839421193\H,-3.9836207687,-3.826
3293224,-6.9039253933\H,-4.2977477632,-5.8268250859,-5.4197658498\H,-4
.1784698535,-5.6000777006,-2.9731712094\C,6.4270066971,-0.1387102643,-
1.9135947103\C,6.5769871455,-1.1341307392,0.7063789541\C,7.4858928584,
-1.5587858897,-0.2589879059\C,7.4139029835,-1.0588559229,-1.5803732654
\H,6.3530072096,0.2520635349,-2.9347756675\H,6.6537980966,-1.545747994
2,1.7164342261\H,8.2578655898,-2.2888480839,0.0075991252\H,8.130313572

7,-1.3989672686,-2.3359930182\O,-3.0376412915,0.9899688544,4.582527355
 1\C,-3.6298886533,2.0166422843,3.7662938582\H,-4.425798878,2.464663176
 8,4.3783386409\H,-2.8870221633,2.7887499307,3.4993713576\H,-4.06443161
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 5.1120508\Quadrupole=-6.5829606,10.3732935,-3.7903329,-22.2834409,-3.2
 983318,-15.5754014\PG=C01 [X(C63H44N1O5P1)]\\@

9-Phen/6 Type II E

1\1\GINC-LOGIN\FOpt\RTPSSTPSS\def2SVP\C63H44N1O5P1\JHIOE\08-Aug-2018\O
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 2147466103\O,-1.3763627412,0.646603154,-1.739957214\O,0.641676735,0.83
 64821493,-0.1746163761\O,0.7631777214,-0.5901893215,-2.4120112526\O,-0
 .5827464747,-1.3562829423,-0.2299932024\C,-1.6002236477,2.5015749034,-
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 ,0.755438275,-0.3695295935\C,-4.1048082367,1.4479515109,0.5818042974\H
 ,-5.0758285483,1.0546097331,0.9012472762\C,-3.6205353745,2.6409464337,
 1.1865687437\C,-2.3357813008,3.1675843806,0.7943674798\C,-1.8227181474
 ,4.2925475226,1.5091546847\H,-0.8299040708,4.6769647892,1.2591755105\C
 ,-2.55430978,4.888890252,2.5260091663\H,-2.1342899983,5.7446822218,3.0
 65770838\C,-3.8394435606,4.3954201675,2.8792965739\H,-4.4089230314,4.8
 800850137,3.6797262501\C,-4.3575167219,3.2908837135,2.2226712859\H,-5.
 335274231,2.882705956,2.5024094545\C,-0.2661420529,2.9879678758,-0.708
 5971875\C,0.8336836043,2.1285312933,-0.6096305842\C,2.171938121,2.5456
 444123,-0.8969901901\C,2.3678890147,3.8371480947,-1.370207819\H,3.3837
 364466,4.1825308956,-1.5910824032\C,1.2763753985,4.727929691,-1.584341
 2075\C,-0.063954134,4.3039789415,-1.2583181821\C,-1.141623881,5.200820
 7875,-1.5283086397\H,-2.1665353204,4.8810116403,-1.3187603296\C,-0.907
 857538,6.4591479722,-2.063300008\H,-1.7518287081,7.127229822,-2.267361
 718\C,0.4153435949,6.8864895112,-2.3549398083\H,0.5865248529,7.8844603
 415,-2.7729671332\C,1.4830840879,6.0339155203,-2.1230357532\H,2.507080
 2842,6.345610335,-2.358326407\C,3.911574342,-3.9372476714,-0.738379856
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9-Phen/6 Type I Z

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9-Phen/6 Type II Z

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7,-2.2854900594\C,5.2013353498,-3.6609580163,-3.068726936\H,5.88329901

63,-4.5086560682,-3.1971274249\H,2.0799933016,-2.5959044713,-3.993191345\H,6.5750011117,-2.6005609308,-1.810380175\H,3.6333201751,-4.5314942997,-4.3095026685\C,-6.6262689354,-0.8874688629,-3.078744929\C,-7.0990801531,-3.2041481216,-1.5650764019\C,-7.4900551308,-1.8628349283,-3.5614502625\C,-7.7274098801,-3.0283608637,-2.7950669962\H,-6.4334901221,0.0219215183,-3.6592331009\H,-7.9861819782,-1.7314953508,-4.529289886\H,-8.4087063972,-3.7997124778,-3.1707480751\H,-7.3013230976,-4.1170202623,-0.9976854911\O,6.8204697339,-1.6899972773,2.509441739\C,7.8889782062,-2.5969364375,2.1935200327\H,8.8025795506,-2.1235648514,2.5811328649\H,7.7382295081,-3.5738399463,2.6873152655\H,7.978943672,-2.7383711433,1.1016072892\\Version=ES64L-G09RevD.01\\State=1-A\\HF=-3198.2560736\\RMSD=6.562e-09\\RMSF=5.289e-06\\Dipole=4.9473201,-1.9423044,4.3744551\\Quadrupole=18.5905445,7.6602762,-26.2508208,-23.7672361,8.5663684,-2.2008475\\PG=C01 [X(C63H44N1O5P1)]\\@

9-Phen/7 Type I E

1\1\GINC-WORKER1\FOpt\RTPSSTPSS\def2SVP\C63H41F3N1O4P1\JHIOE\13-Mar-2018\0\#p tpsstps\def2svp empiricaldispersion=gd3 int=ultrafine opt sc rf=(smd,solvent=ch2cl2,read)\\title\0,1\P,0.0049056209,-0.2558747485,-1.2686982256\O,-1.3303999485,0.6599455365,-1.7095168191\O,0.7280184618,0.8694648485,-0.2208712288\O,0.8217791305,-0.4748029618,-2.5061656631\O,-0.4153367211,-1.3729039102,-0.3161287715\C,-1.4863767267,2.5599967737,-0.2611370334\C,-2.0216866339,1.357745084,-0.7386448904\C,-3.271074681,0.8265145379,-0.2824194435\C,-3.9875951879,1.5609621248,0.655389943\H,-4.9575961803,1.191679554,1.0045888451\C,-3.4826946001,2.773171667,1.2037812221\C,-2.1979029835,3.2694669261,0.7729183982\C,-1.6677054778,4.420494232,1.4317666082\H,-0.674888495,4.7852597248,1.1548254914\C,-2.3859473519,5.0725911606,2.4232765954\H,-1.9535833634,5.9492234449,2.9180643121\C,-3.672662908,4.6102770875,2.809092937\H,-4.2298920576,5.1363414917,3.5916989928\C,-4.2044714742,3.4790624336,2.2130591371\H,-5.1789849204,3.0888830485,2.5259287154\C,-0.1620263305,3.0225224776,-0.7716330735\C,0.9269331477,2.1498242938,-0.6896162672\C,2.2596716806,2.5236267311,-1.0471572108\C,2.4645293598,3.7945954254,-1.5663965447\H,3.4761860858,4.1091978091,-1.8445123062\C,1.3828402092,4.7047174814,-1.75438625\C,0.0472578195,4.3208910276,-1.3617184983\C,-1.0194447434,5.2363168033,-1.6112309529\H,-2.0418962414,4.9459878469,-1.3525612162\C,-0.7793957187,6.4759345565,-2.1857440864\H,-1.6156007038,7.1589446358,-2.3715497384\C,0.539771407,6.8644628017,-2.5420583617\H,0.716343922,7.8477287688,-2.9915704785\C,1.5961083094,5.9916091485,-2.3343889232\H,2.616126828,6.2727759937,-2.6200913929\C,-1.791689709,0.0055059312,4.3474269225\C,-1.4523229594,-1.2234976872,4.9360477693\H,-1.9760778336,-1.5682873302,5.8315394301\C,-0.4398429912,-2.0055693177,4.3720593081\H,-0.181721455,-2.9625464061,4.8345725719\C,0.2107921311,-1.5817811139,3.1918289118\C,-0.1302774918,-0.3375695935,2.6159294332\H,0.3885582584,0.0262733204,1.7265975277\C,-1.1204188467,0.4558159229,3.1979817671\H,-1.3753470036,1.4205032931,2.74961818\C,1.2626602165,-2.4335181195,2.5906568531\C,2.2127584344,-3.1569983229,3.4930824063\H,3.1646883606,-3.3779785173,2.9869582232\H,1.7660237808,-4.1152146678,3.8177275818\H,2.3974729615,-2.5532282724,4.3947134933\N,1.3295574229,-2.4990160406,1.2838215376\H,0.5894184468,-1.9657620911,0.6823720023\C,2.2415382951,-3.2514965421,0.478876739\C,2.7799204218,-2.6119318112,-0.6538061042\H,2.5378319037,-1.5691435316,-0.8710026605\C,3.647378383,-3.3186871894,-1.4945423512\H,4.0774499239,-2.8116492272,-2.3640012499\C,3.9667889569,-4.6575540548,-1.2204162998\C,3.4038488431,-5.2969107996,-0.1043725161\H,3.6311914242,-6.3480478537,0.1017422295\C,2.5351450255,-4.6021943333,0.7478546433\H,2.0665574323,-5.1142791518,1.5919094899\H,4.64672704

97,-5.2050402381,-1.8815340047\C,-2.9224740023,0.8336070805,4.9057469843\C,-3.7699365796,-0.4732995071,-0.8194496548\C,-4.0294529008,-1.6008429216,0.0635407917\C,-3.9737411467,-0.6117566456,-2.1749083903\C,-3.7715133008,-1.5261958506,1.4609013254\C,-4.5279630572,-2.8352079836,-0.4830620223\C,-4.4603272267,-1.8271086974,-2.7600824949\H,-3.7634188401,0.2310570682,-2.8411329893\C,-4.0189928374,-2.6019545831,2.3047088606\H,-3.3612420626,-0.6038164331,1.8761707179\C,-4.7747328474,-3.915641962,0.4084946154\C,-4.7505363211,-2.9545123783,-1.9219506633\C,-4.5327765752,-3.8063450435,1.7740220454\H,-3.8116064116,-2.5104948871,3.3762488956\H,-5.1609882121,-4.8609062279,0.0166741601\H,-4.7343823627,-4.6579691241,2.4330234399\C,3.3697680645,1.5395162491,-0.8830108535\C,3.7312799046,1.0325549305,0.4318698837\C,4.0391348968,1.0841783408,-1.9967347907\C,3.0835349852,1.5011464352,1.6086985845\C,4.7637139587,0.0397868144,0.5555787741\C,5.0832528423,0.1017247413,-1.914538537\H,3.7462289326,1.4467475922,-2.9876961245\C,3.4051349705,0.9972476887,2.8631124674\H,2.3127367937,2.2725345303,1.5203157257\C,5.0654467107,-0.4595748286,1.8526283182\C,5.4602528667,-0.432855752,-0.6382450818\C,4.4003392614,0.0011256262,2.9844507683\H,2.8845656646,1.3684905938,3.7523382814\H,5.8366834595,-1.2255219571,1.9717204665\H,4.65343799,-0.4068066489,3.9690423907\C,-5.2341657576,-4.1396041637,-2.5404042504\C,-4.6607322892,-1.9232972017,-4.1659211871\C,-5.1335467835,-3.0965328909,-4.7404706047\C,-5.421699884,-4.2115711916,-3.9181255122\H,-4.4329753318,-1.0508751449,-4.7889113844\H,-5.2827451224,-3.1603151364,-5.8238734385\H,-5.7942304779,-5.1389326788,-4.3669588749\H,-5.4637209051,-5.0187152388,-1.9316624554\C,5.726765742,-0.3688308516,-3.0931809337\C,6.4838859452,-1.4175415065,-0.6021734136\C,7.1027733758,-1.8609915989,-1.7677116306\C,6.7216081246,-1.3371166066,-3.025327719\H,5.418646597,0.0451303044,-4.0598478548\H,6.7945466409,-1.8478368522,0.3538873185\H,7.886311119,-2.6242711122,-1.7084955145\H,7.2079157614,-1.6944367743,-3.939472188\F,-2.6181992713,2.1550840679,4.9435040066\F,-3.2708577346,0.465064887,6.1615285258\F,-4.0464717508,0.7169759983,4.1388821606\\Version=ES64L-G09RevD.01\\State=1-A\\HF=-3420.6107591\\RMSD=4.113e-09\\RMSF=6.579e-06\\Dipole=2.7169517,-3.0533205,4.2266188\\Quadrupole=-12.2672717,18.0144115,-5.7471397,-17.6475533,4.4322221,-21.7471267\\PG=C01 [X(C63H41F3N1O4P1)]\\@

9-Phen/7 Type II E

1\\1\\GINC-WORKER0\FOpt\RTPSSSTPSS\def2SVP\C63H41F3N1O4P1\JHIOE\13-Mar-2018\\#p tpsstps\def2svp empiricaldispersion=gd3 int=ultrafine opt sc rf=(smd,solvent=ch2cl2,read)\\title\\0,1\\P,-0.082343997,-0.2646760938,-1.258740287\\O,-1.3847061152,0.6635688305,-1.7667313134\\O,0.6249697835,0.867418586,-0.1962205813\\O,0.7775429249,-0.5200293316,-2.4590967206\\O,-0.5512289709,-1.3475061893,-0.2901487907\\C,-1.6210154371,2.522346565,-0.2823855265\\C,-2.1198873578,1.3223441753,-0.799491711\\C,-3.3544323398,0.7415657107,-0.3697563377\\C,-4.0943136212,1.4208458603,0.5902849208\\H,-5.0504880407,1.0072687515,0.9282333779\\C,-3.624962626,2.6273201522,1.1817306132\\C,-2.3573356597,3.1795615516,0.7678394645\\C,-1.8593904985,4.3197381496,1.4693155594\\H,-0.8787529607,4.7246941359,1.2047278501\\C,-2.5900113566,4.9069636718,2.4920337686\\H,-2.1815685873,5.7759481829,3.0194769355\\C,-3.8588626809,4.3881914127,2.8662512124\\H,-4.4281477825,4.8660433381,3.6708585504\\C,-4.3611155713,3.2679719229,2.2240995377\\H,-5.3262468485,2.8411570857,2.519500106\\C,-0.2898411617,3.0152389903,-0.7437751467\\C,0.8114742601,2.1612056029,-0.6343676316\\C,2.1515942788,2.5783938568,-0.9047148319\\C,2.3554368363,3.8636305086,-1.3856063894\\H,3.3735910936,4.209243955,-1.5944689478\\C,1.2626626737,4.7516674353,-1.6147050497\\C,-0.080924472,4.3300411614,-1.2942016224\\C,-1.15584093

78,5.228744434,-1.5673596543\H,-2.181428799,4.9096976737,-1.3592564199
\C,-0.918523775,6.4871836998,-2.1003050977\H,-1.7604034846,7.157363425
,-2.306068443\C,0.4063191451,6.9114079605,-2.3884080299\H,0.5807376166
,7.9096285075,-2.8044472699\C,1.4720925298,6.0570838574,-2.1527327624\
H,2.4971771019,6.3686020735,-2.3835467567\C,3.616133527,-4.0100629897,
-1.0736269828\C,3.4993500978,-4.773766091,0.1042641891\H,3.9171782213,
-5.7841715277,0.149719179\C,2.8429084116,-4.240918095,1.2147034087\H,2
.7396660846,-4.8448399672,2.1206831353\C,2.2829474887,-2.9423733923,1.
1529645659\C,2.4355209848,-2.1799909565,-0.0230697426\H,2.100153146,-1
.1420797298,-0.0520141364\C,3.0879693887,-2.7139846385,-1.137150579\H,
3.185281116,-2.1104057035,-2.0411016845\C,1.565052771,-2.3885033605,2.
3208488065\C,2.0666230097,-2.6893236705,3.6988279871\H,1.7848572997,-1
.8994453831,4.4117623139\H,3.1603447801,-2.8051676688,3.6789533991\H,1
.6320082821,-3.6421248439,4.054764066\N,0.5168292249,-1.6340739822,2.0
914663848\H,0.1677580753,-1.5064878961,1.0652662354\C,-0.3297584208,-0
.9770909987,3.0395811864\C,-0.7093939999,0.3470039368,2.7460686626\H,-
0.3314671197,0.824772697,1.8385021529\C,-1.5675556772,1.0246551447,3.6
201001878\H,-1.8540843713,2.0573094668,3.3991729067\C,-2.06704346,0.38
06324009,4.7639124269\C,-1.7073318572,-0.9494828019,5.0321372012\H,-2.
1127138857,-1.4647202757,5.909099622\C,-0.8389177849,-1.6370474666,4.1
7297119\H,-0.5938601162,-2.6849789001,4.3613629835\H,-2.7462051959,0.9
12081029,5.4387482858\C,4.3437060528,-4.6038684701,-2.2550035011\C,-3.
8086490295,-0.5595357483,-0.9436760163\C,-3.9723032507,-1.7312227579,-
0.0970338959\C,-4.0662973694,-0.6533721906,-2.2935181528\C,-3.64104989
01,-1.7005846614,1.2869369527\C,-4.4434055406,-2.9638155141,-0.6705461
376\C,-4.5326262813,-1.8643291317,-2.9047238911\H,-3.9228816238,0.2230
575424,-2.9341514945\C,-3.7921152413,-2.8226762264,2.0928852082\H,-3.2
41374636,-0.7787938466,1.7171705557\C,-4.5897510141,-4.0920170759,0.18
32346709\C,-4.7391092519,-3.0335041706,-2.0996054298\C,-4.2784422309,-
4.0273117326,1.5371714656\H,-3.525073026,-2.7712480584,3.1536825731\H,
-4.9481416099,-5.0393668236,-0.2291597389\H,-4.4016822502,-4.914803646
3,2.1676087441\C,3.2668895382,1.6196730181,-0.6493147376\C,3.570944080
7,1.1998132203,0.7098924553\C,3.9784127706,1.0941479149,-1.7029673567\
C,2.8609226149,1.7312216356,1.8222408075\C,4.5982098509,0.2220633787,0
.9419465541\C,5.0054067091,0.107630335,-1.5141948551\H,3.727629092,1.3
928851618,-2.7261685845\C,3.1295683332,1.3132309996,3.1200883832\H,2.0
842694434,2.48194952,1.6476192359\C,4.8513922961,-0.1819495905,2.28148
97841\C,5.3230274882,-0.3466748884,-0.1913431077\C,4.1338286716,0.3460
677201,3.350451351\H,2.5618470114,1.730756362,3.9585570565\H,5.6237694
103,-0.9287227833,2.4848667248\H,4.3492298097,0.0090075676,4.370122349
9\C,5.6705954718,-0.4651197271,-2.6335434477\C,6.3032526208,-1.3654443
318,-0.051495128\C,6.9339134763,-1.9190602749,-1.1619656559\C,6.617375
3805,-1.4677157837,-2.4645510677\H,7.1074726278,-1.9172946971,-3.33456
57969\H,7.6714238617,-2.7168631283,-1.025175255\H,5.4067405459,-0.1129
786864,-3.6371249574\H,6.5630982342,-1.7407680074,0.9421307503\C,-4.80
11492147,-1.9131932236,-4.3015747228\C,-5.2154497548,-4.2094446895,-2.
7406585268\C,-5.4719048805,-4.2345212286,-4.1088787314\H,-5.8371835052
,-5.1564945643,-4.5745058686\C,-5.2633556801,-3.0792880334,-4.89900385
21\H,-4.6339929803,-1.0098528145,-4.8992080666\H,-5.46516871,-3.106586
1516,-5.9754103879\H,-5.3872746458,-5.1184775498,-2.1574254995\F,5.642
6519648,-4.8849463156,-1.9551786322\F,3.7833332225,-5.7779957769,-2.65
13707481\F,4.355245385,-3.7843113105,-3.331709085\\Version=ES64L-G09Re
vD.01\State=1-A\HF=-3420.610945\RMSE=4.029e-09\RMSF=2.856e-06\Dipole=0
.7878101,-1.1166939,6.0527803\Quadrupole=-16.5993857,6.4946772,10.1047
085,-8.3174379,2.7840429,-21.5135758\PG=C01 [X(C63H41F3N1O4P1)]\@

9-Phen/7 Type I Z

1\1\GINC-WORKER1\SP\RTPSSTPSS\def2SVP\C63H41F3N1O4P1\JHIOE\22-Aug-2018

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\0\#p tpsstps\def2svp int=ultrafine empiricdispersion=gd3 scrf=(sm
d,externaliteration,dovacuum,read,solvent=ch2cl2)\title\0,1\P,0,-1.5
837,-0.570412,-1.262423\O,0,-2.654348,0.713033,-1.366834\O,0,-0.19122,
0.27781,-0.773951\O,0,-1.441721,-1.153972,-2.638113\O,0,-1.918105,-1.4
13659,-0.030793\C,0,-1.760198,2.492867,-0.055379\C,0,-2.739424,1.51559
9,-0.241263\C,0,-3.805148,1.287952,0.684997\C,0,-3.864326,2.097291,1.8
13884\H,0,-4.676944,1.958169,2.534944\C,0,-2.876856,3.087309,2.080623\
C,0,-1.791604,3.282582,1.149861\C,0,-0.761883,4.207804,1.500607\H,0,0.
092038,4.337308,0.830163\C,0,-0.82199,4.931544,2.682588\H,0,-0.015993,
5.630679,2.931097\C,0,-1.914725,4.769921,3.576143\H,0,-1.952934,5.3528
22,4.502734\C,0,-2.917855,3.86136,3.280337\H,0,-3.754797,3.710089,3.97
1437\C,0,-0.654807,2.616775,-1.049199\C,0,0.137762,1.49527,-1.332054\C
,0,1.341493,1.587781,-2.107756\C,0,1.648294,2.813196,-2.691312\H,0,2.5
5554,2.905866,-3.297708\C,0,0.80293,3.948752,-2.553763\C,0,-0.366754,3
.860071,-1.715607\C,0,-1.214173,5.004738,-1.612785\H,0,-2.120474,4.944
268,-1.002872\C,0,-0.913006,6.178647,-2.28743\H,0,-1.583325,7.041006,-
2.20157\C,0,0.251906,6.270329,-3.09666\H,0,0.478354,7.204465,-3.622159
\C,0,1.090395,5.174974,-3.226801\H,0,1.985904,5.228542,-3.856303\C,0,4
.883248,-0.13001,2.667119\C,0,3.954502,0.290119,3.634242\H,0,4.293893,
0.805555,4.537385\C,0,2.591118,0.055566,3.432517\H,0,1.870815,0.387875
,4.185233\C,0,2.149774,-0.621147,2.274102\C,0,3.094999,-1.035344,1.308
146\H,0,2.767982,-1.516437,0.38319\C,0,4.453733,-0.792506,1.506002\H,0
,5.176499,-1.101672,0.747919\C,0,0.706758,-0.781562,1.996348\C,0,-0.23
3287,0.328703,2.342547\H,0,-1.205989,0.191103,1.849404\H,0,0.200049,1.
303083,2.070478\H,0,-0.386024,0.328958,3.439262\N,0,0.21123,-1.838906,
1.400887\H,0,-0.763417,-1.709579,0.937947\C,0,0.837297,-3.091105,1.122
887\C,0,0.598658,-3.6844,-0.130697\H,0,-0.033948,-3.178267,-0.864718\C
,0,1.197713,-4.915377,-0.428586\H,0,1.029055,-5.370466,-1.409481\C,0,2
.011834,-5.556078,0.518139\C,0,2.215309,-4.970388,1.779473\H,0,2.83022
6,-5.47809,2.529894\C,0,1.627272,-3.73957,2.091047\H,0,1.770562,-3.285
206,3.075633\H,0,2.479503,-6.516849,0.278806\C,0,6.344204,0.20659,2.83
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