

Internal Acidity Scale and Reactivity Evaluation of Chiral Phosphoric Acids with Different 3,3'-Substituents in Brønsted Acid Catalysis

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1. Experimental data

1.1 Chemistry

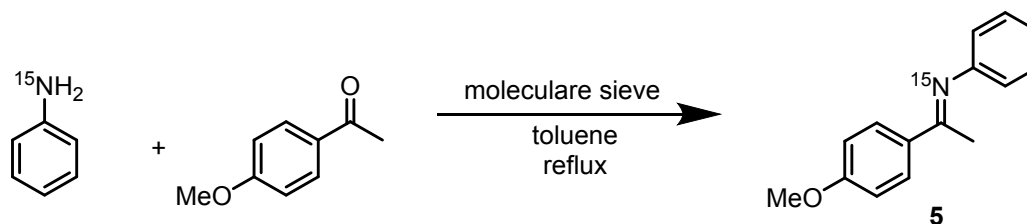
Deuterated solvents were purchased from Deutero or Sigma Aldrich. When anhydrous solvents were required, CD_2Cl_2 was freshly distilled over CaH_2 under argon atmosphere. The catalysts were purchased from Sigma Aldrich or synthesized from the corresponding binaphthols according to the procedure of Klusmann et al.¹

1.2 Synthesis of Imine Substrates

The imines were prepared according to a modified literature procedure.²⁻⁷ 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. For the preparation of imines **10-13** see reference.²

1.2.1 Exemplary procedure for (E)-1-(4-methoxyphenyl)-N-phenylethan-1-imine (98% ^{15}N) **5**

For the syntheses of the imines, the same procedure was used as in our previous publication.²



Molecular sieves 4 Å (1.625 g) were weighed into a 25 ml Schlenk flask equipped with a reflux condenser and a stopper. The setup was connected to a vacuum line and was evacuated and dried with a heat gun. 4-Methoxyacetophenone (0.500 g, 3.33 mmol) and Aniline (98% ^{15}N , 0.31 ml, 0.316 g, 3.35 mmol) were added to the Schlenk flask under argon atmosphere and were dissolved in 5 ml toluene. The stop cock was exchanged with a drying tube filled with CaCl_2 and the solution was heated to reflux overnight. The orange solution was filtered off from the molecular sieves and was concentrated under reduced pressure. The remaining solid was recrystallized from methanol. The product was obtained as yellow solid (0.303 g, 1.33 mmol, 40%) and predominantly as *E*-isomer (>99 % via ^1H -NMR analysis).

^1H -NMR (400.1 MHz, CD_2Cl_2) δ_{H} = 7.95 (m, 2H, Aryl-H), 7.35 (m, 2H, Aryl-H), 7.07 (m, 1H, Aryl-H), 6.96 (m, 2H, Aryl-H), 6.77 (m, 2H, Aryl-H), 3.86 (s, 3H, $-\text{OCH}_3$), 2.18 ppm (d, $^3J_{\text{HN}}$ = 1.76 Hz, $-\text{CH}_3$)

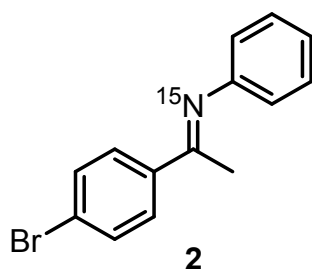
^{13}C -NMR {1H} (100.6 MHz, CD_2Cl_2): δ_{C} = 164.5 (d, $^1J_{\text{NC}}$ = 7.1 Hz), 161.9, 152.5 (d, $^2J_{\text{NC}}$ = 1.7 Hz), 132.5 (d, $^1J_{\text{NC}}$ = 8.4 Hz), 129.3, 129.2 (d, $^3J_{\text{NC}}$ = 3.3 Hz), 123.2, 119.9 (d, $^2J_{\text{NC}}$ = 2.3 Hz), 113.9, 55.8, 17.2 ppm (d, $^2J_{\text{NC}}$ = 2.7 Hz)

^{15}N -NMR (40.5 MHz, CD_2Cl_2): δ_{N} = 325.5 ppm

^1H - and ^{13}C -spectra were in accordance with the literature.⁸

1.2.2 (E)-1-(4-bromophenyl)-N-phenylethan-1-imine (98 % ¹⁵N) 2

For the syntheses of the imines, the same procedure was used as in our previous publication.²



The reaction was carried out on 4.32 mmol scale.

The remaining yellow-orange residue was dissolved in 1 ml MeOH under gentle heating (water bath 60°C) and was stored in the fridge (~ 4°C). The crystallized product was sucked off over a Büchner funnel and was washed with ice-cold MeOH. Solvent residues were removed under reduced pressure. The product was obtained as almost yellow crystalline solid (0.438 g, 38 %) and predominantly as *E*-isomer (~ 99% via ¹H-NMR analysis).

¹H-NMR (400.1 MHz, CD₂Cl₂) δ_H = 7.87 (2H, m, Aryl-H), 7.59 (2H, m, Aryl-H), 7.36 (2H, m, Aryl-H), 7.09 (1H, m, Aryl-H), 6.77 (2H, m, Aryl-H), 2.20 ppm (3H, d, ³J_{NH} = 1.8 Hz, -CH₃)

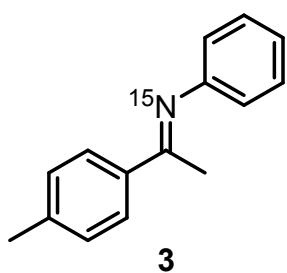
¹³C-NMR {1H} (100.6 MHz, CD₂Cl₂): δ_C = 164.5 (d, ¹J_{CN} = 7.2 Hz), 151.9 (¹J_{CN} = 1.5 Hz), 138.9 (d, ²J_{CN} = 8.6 Hz), 131.8, 129.3, 129.2 (d, 3.3 Hz), 125.2, 123.6, 119.6 (2.3 Hz), 17.3 (d, ²J_{CN} = 2.8 Hz)

¹⁵N-NMR (40.5 MHz, CD₂Cl₂): δ_N = 333.4 ppm

¹H- and ¹³C-spectra were in accordance with the literature.⁹

1.2.3 (E)-1-(4-methylphenyl)-N-phenylethan-1-imine (98% ¹⁵N) 3

For the syntheses of the imines, the same procedure was used as in our previous publication.²



The reaction was carried out on 3.73 mmol scale.

The solidified residue was washed with cooled MeOH (~-35°C). After drying under reduced pressure over CaCl₂, the product was obtained as orange crystals (0.220 g, 1.05 mmol, 28 %) predominantly as *E*-isomer (>99 % via ¹H-NMR analysis). The product was used without further purification.

¹H-NMR (400.1 MHz, CD₂Cl₂) δ_H = 7.87 (m, 2H, Aryl-H), 7.34 (m, 2H, Aryl-H), 7.26 (m, 2H, Aryl-H), 7.07 (m, 1H, Aryl), 6.76 (m, 2H), 2.41 (s, 3H, -CH₃), 2.19 ppm (d, ³J_{HN} = 1.76 Hz, 3H, -CH₃)

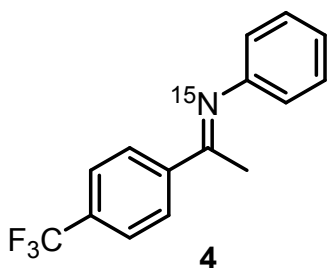
¹³C-NMR {1H} (100.6 MHz, CD₂Cl₂): δ_C = 165.3, 152.4, 141.2, 133.9, 129.5, 129.3, 127.5, 123.3, 119.7, 21.5, 17.4 ppm

¹⁵N-NMR (40.5 MHz, CD₂Cl₂): δ_N = 328.9 ppm

¹H- and ¹³C-spectra were in accordance with the literature.⁵

1.2.4 (E)-N-phenyl-1-(4-(trifluoromethyl)phenyl)ethan-1-imine (98% ¹⁵N) 4

For the syntheses of the imines, the same procedure was used as in our previous publication.²



The reaction was carried out on 1.59 mmol scale.

The obtained yellow solid was further dried in the desiccator over KOH. The product was obtained as yellow solid (0.306, 1.16 mmol, 72 %) predominantly as *E*-isomer (>99 % via ¹H-NMR analysis). The product was used without further purification.

¹H-NMR (400.1 MHz, CD₂Cl₂): δ_H = 8.11 (m, 2H, Aryl-H), 7.73 (m, 2H, Aryl-H), 7.38 (m, 2H, Aryl-H), 7.12 (m, 1H, Aryl-H), 6.80 (m, 2H, Aryl-H), 2.25 ppm (d, ³J_{NH} = 1.8 Hz, 3H, -CH₃)

¹³C-NMR {1H} (100.6 MHz, CD₂Cl₂): δ_C = 164.5, 152.0, 143.2, 132.1, 129.4, 128.0, 125.6, 124.6, 123.9, 119.5, 17.5 ppm

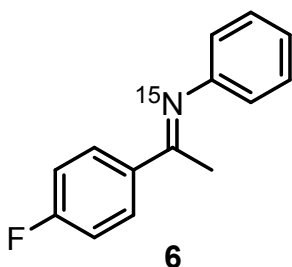
¹⁹F-NMR {1H} (376 MHz, CD₂Cl₂): δ_F = - 63.1 ppm

¹⁵N-NMR (60.8 MHz, CD₂Cl₂): δ_N = 338.2 ppm

¹H- and ¹³C-spectra were in accordance with the literature.⁵

1.2.5 (E)-1-(4-fluorophenyl)-N-phenylethan-1-imine (98 % ¹⁵N) 6

For the syntheses of the imines, the same procedure was used as in our previous publication.²



The reaction was carried out on 4.32 mmol scale.

The remaining yellow-orange residue was dissolved in 1 ml MeOH under gentle heating (water bath 60°C) and was stored in the fridge (~ 4°C). The crystallized product was washed with ice-cold MeOH. Solvent residues were removed under reduced pressure. The product was obtained as almost colorless/slightly yellowish crystalline solid (0.248 g, 27 %) and predominantly as *E*-isomer (~ 99% via ¹H-NMR analysis).

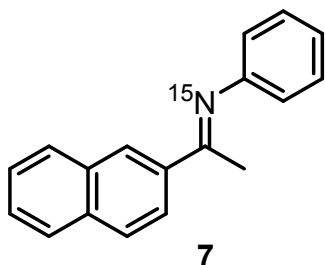
¹H-NMR (400.1 MHz, CD₂Cl₂) δ_H = 8.00 (2H, m, Aryl-H), 7.35 (2H, m, Aryl-H), 7.14 (2H, m, Aryl-H), 7.09 (1H, m, Aryl-H), 6.77 (2H, m, Aryl-H), 2.20 ppm (3H, d, ³J_{NH} = 1.8 Hz, -CH₃)

¹³C-NMR {1H} (100.6 MHz, CD₂Cl₂): δ_C = 164.6, 164.3, 152.1, 136.2, 129.7, 129.3, 123.5, 119.6, 115.5, 17.4 ppm

¹⁵N-NMR (40.54 MHz, CD₂Cl₂): δ_N = 330.9 ppm

¹H- and ¹³C-spectra were in accordance with the literature.⁸

1.2.6 (E)-1-(naphthalen-2-yl)-N-phenylethan-1-imine (98% ¹⁵N) 7



For the syntheses of the imines, the same procedure was used as in our previous publication.²

The reaction was carried out on 4.33 mmol scale.

The intensive orange solution was cooled down and was quickly filtered off from the molecular sieves. The product started crystallizing at r.t. Crystallization was completed in an ice bath for 2 h. The yellow crystals were sucked off with a Büchner funnel and were washed with ice-cold toluene. The liquid residue was concentrated under reduced pressure and the resulting solid was suspended in 2.5 ml methanol and was shortly heated at 60°C in a water bath. After cooling down, the yellow solid was sucked off with a Büchner funnel and washed with ice cold methanol. Solvent residues were removed under reduced pressure. The product was obtained as yellow solid (0.489 g, 1.99 mmol, 45 % yield) predominantly as *E*-isomer (>99 % via ¹H-NMR analysis).

¹H-NMR (400.1 MHz, CD₂Cl₂) δ_H = 8.37 (s, 1H, Aryl-H), 8.24 (dd, ³J_{HN} = 8.68 Hz, ⁴J = 1.64 Hz, 1H, Aryl-H) 7.99 – 7.94 (m, 1H, Aryl-H), 7.94 – 7.87 (m, 2H, Aryl-H), 7.60 – 7.52 (m, 2H, Aryl-H), 7.42 – 7.35 (m, 2H, Aryl-H), 7.11 (m, 1H, Aryl-H), 6.83 (m, 2H, Aryl-H), 2.34 ppm (d, ³J_{HN} = 1.76 Hz, 3H, -CH₃)

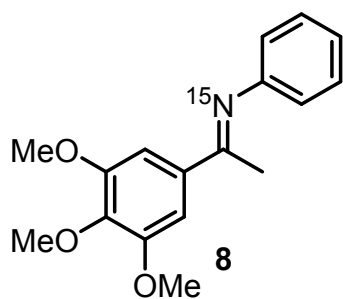
¹³C-NMR {1H} (100.6 MHz, CD₂Cl₂): δ_C = 165.3, 152.3, 137.3, 134.8, 133.3, 129.3, 129.2, 128.2, 128.1, 128.0, 127.6, 126.7, 124.6, 123.5, 119.7, 17.4 ppm

¹⁵N-NMR (40.5 MHz, CD₂Cl₂): δ_N = 333.5 ppm

¹H- and ¹³C-spectra were in accordance with the literature.⁸

1.2.7 (E)-N-phenyl-1-(3',4',5'-(trimethoxy)phenyl)ethan-1-imine (98% ¹⁵N) 8

For the syntheses of the imines, the same procedure was used than in our previous publication.²



To the mixture of 3,4,5-Trimethoxyacetophenone (0.486 g, 2.30 mmol) and Aniline (98% ¹⁵N, 0.22 ml, 2.30 mmol) additionally sodium bicarbonate (1g, 11.9 mmol) was added. The reaction was carried out in 2.30 mmol scale.

The solidified residue was washed with cooled MeOH (~-35°C). After drying under reduced pressure, the product was obtained as colorless solid (0.140 g, 0.49 mmol, 21 %) predominantly as *E*-isomer (>99 % via ¹H-NMR analysis). The product was used without further purification.

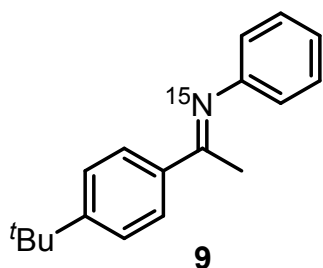
¹H-NMR (400.1 MHz, CD₂Cl₂) δ_H = 7.35 (m, 2H, Aryl-H), 7.24 (s, 2H, Aryl-H), 7.08 (m, 1H, Aryl-H), 6.76 (m, 2H, Aryl-H), 3.91 (s, 6H, OCH₃), 3.83 (s, 3H, -OCH₃), 2.19 ppm (d, ³J_{HN} = 1.75 Hz, 3H, -CH₃)

¹³C-NMR {1H} (100.6 MHz, CD₂Cl₂): δ_C = 164.9, 153.8, 152.3, 140.8, 135.5, 129.7, 123.8, 120.0, 105.4, 61.4, 56.9, 17.8

¹⁵N-NMR (40.5 MHz, CD₂Cl₂): δ_N = 329.7 ppm

1.2.8 (E)-N-phenyl-1-(4-(tert-butyl)phenyl)ethan-1-imine (98% ¹⁵N) 9

For the syntheses of the imines, the same procedure was used than in our previous publication.²



The reaction was carried out in 2.84 mmol scale.

The solidified residue was recrystallized in 0,4 ml ethanol and washed with cooled MeOH (~-35°C). After drying under reduced pressure, the product was obtained as colorless crystals (0.160 g, 0.63 mmol, 22 %) predominantly as *E*-isomer (>99 % via ¹H-NMR analysis). The product was used without further purification.

¹H-NMR (400.1 MHz, CD₂Cl₂) δ_H = 7.91 (m, 2H, Aryl-H), 7.48 (m, 2H, Aryl-H), 7.35 (m, 2H, Aryl-H), 7.07 (m, 1H, Aryl-H), 6.76 (m, 2H, Aryl-H), 2.20 (d, ³J_{HN} = 1.83 Hz, 3H, -CH₃), 1.34 (s, 9H, *tert*-Butyl)

¹³C-NMR {¹H} (100.6 MHz, CD₂Cl₂): δ_C = 165.9, 154.9, 153.1, 137.9, 129.6, 128.0, 126.3, 124.0, 120.4, 35.7, 32.0, 18.1 ppm

¹⁵N-NMR (40.5 MHz, CD₂Cl₂): δ_N = 329.4 ppm

¹H- and ¹³C-spectra were in accordance with the literature.⁵

1.3 Sample preparation of binary complexes in CD₂Cl₂

The catalyst was dried for 30 min at 150°C under reduced pressure. Ketimine and phosphoric acid catalyst were directly weighed into a 5 mm NMR tube under an inert argon atmosphere. CD₂Cl₂ (0.6 ml) and 1.0 ml of tetramethylsilane atmosphere were added to the tube. The sample was stored in an -80°C freezer. For all samples a 1:1 ratio of catalyst/ketimine was used. Even after careful sample preparation, partial hydrolysis of the imine could not be completely prevented. Therefore the imine/CPA-ratios are slightly different from 1:1. A concentration of 25 mmol or 50 mmol/L was used for all samples, depending on solubility at low temperatures.

2 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 $^1\text{H}/^{31}\text{P}$ and a 5 mm CPPBBO BB- $^1\text{H}/^{19}\text{F}$. Triple resonance experiments were performed on the TBI probe head. The temperature was controlled in the VT-experiments by BVT 3000 and BVTE 3900. For NMR measurements employing standard NMR solvents, 5 mm NMR tubes were used, if not otherwise noted. NMR data were processed, evaluated and plotted with TopSpin 3.2 software. Further plotting of the spectra was performed with Corel Draw X7, X8 or 2017 software. ^1H and ^{13}C chemical shifts were referenced to TMS or the respective solvent signals. The heteronuclear ^{15}N and ^{19}F spectra were referenced, employing $\nu(X) = \nu(\text{TMS}) \times \Xi_{\text{reference}} / 100 \%$ according to Harris *et al.*¹⁰ 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)

2.1 Pulse programs

All pulse programs used are standard Bruker NMR pulse programs.

2.2 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;

^{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;

^{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;

^{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;

3 Steiner-Limbach correlation

3.1 Theory

All investigations regarding the hydrogen bond analysis were done in accordance with our previous work on TRIP/imine complexes.²

The ¹H and ¹⁵N chemical shifts of an OHN hydrogen bond can be correlated by multiplication of the constants $\delta(\underline{\text{OH}})^\circ$, $\delta(\underline{\text{HN}})^\circ$, $\delta(\underline{\text{HN}})^\circ$ and $\delta(\underline{\text{N}})^\circ$ with the defined valence bond orders p_{OH}^{H} (equation S1 and S2). $\delta(\underline{\text{OH}})^\circ$, $\delta(\underline{\text{HN}})^\circ$, $\delta(\underline{\text{HN}})^\circ$ and $\delta(\underline{\text{N}})^\circ$ reflect the ¹H respectively ¹⁵N chemical shifts of the isolated diatomic units.^{11,12}

$$\delta(\underline{\text{OHN}}) = \delta(\underline{\text{OH}})^\circ p_{\text{OH}}^{\text{H}} + \delta(\underline{\text{HN}})^\circ p_{\text{HN}}^{\text{H}} + 4 \delta(\underline{\text{OHN}})^* p_{\text{OH}}^{\text{H}} p_{\text{HN}}^{\text{H}} \quad (\text{S1})$$

$$\delta(\underline{\text{OHN}})_{\text{ref}} = \delta(\underline{\text{N}})^\circ p_{\text{OH}}^{\text{H}} + \delta(\underline{\text{HN}})^\circ p_{\text{HN}}^{\text{H}} + 4 \delta(\underline{\text{OHN}})^* p_{\text{OH}}^{\text{H}} p_{\text{HN}}^{\text{H}} \quad (\text{S2})$$

$\delta(\underline{\text{HN}})^\circ$ and $\delta(\underline{\text{HN}})^\circ$ are the ¹⁵N, respectively ¹H chemical shift of the completely protonated imine and are experimentally accessible. $\delta(\underline{\text{OH}})^\circ$ is the chemical shift of the free phosphoric acid (CPA). Because of dimerization and remaining water, $\delta(\underline{\text{OH}})^\circ$ has to be fitted. $\delta(\underline{\text{N}})^\circ$ takes into account the referencing of the ¹⁵N chemical shift (see chapter 3.2). To consider the asymmetry of the OHN hydrogen bond compared to symmetric XHX hydrogen bond, the correction factors $\delta(\underline{\text{OHN}})^*$ and $\delta(\underline{\text{OHN}})^*$ are used (for values see table S1). These parameters were slightly modified compared to our previous publication.²

Table S 1: NMR parameters used for the hydrogen-bond correlations.

systems	$\delta(\underline{\text{N}})^\circ$ [ppm]	$\delta(\underline{\text{HN}})^\circ$ [ppm]	$\delta(\underline{\text{OHN}})^*$ [ppm]	$\delta(\underline{\text{OH}})^\circ$ [ppm]	$\delta(\underline{\text{HN}})^\circ$ [ppm]	$\delta(\underline{\text{OHN}})^*$ [ppm]
pyridine–HA ¹¹ in CDF ₃ /CDF ₂ Cl	0	126	-4	2	7	20
collidine–HA ¹¹ in CDF ₃ /CDF ₂ Cl	0	126	-8	2	7	20
solid collidine–HA ¹³	0	126	0	-3	7	20
imine/TRIP ²	0	-170	-6	2	6	16
imine/TiPSY, imine/TRIFP and imine/TRIM	0	-151.6	-4.89	1.04	12.33	14.2

To consider the zero anharmonic vibrations of the hydrogen atom within the hydrogen bond Limbach and Denisov proposed the correction factors for the valence bond orders p_{OH}^{H} and p_{NH}^{H} (equation S3 and S4).^{11,12,14} For explanation and details of these terms see reference.¹⁴

$$p_{\text{OH}}^{\text{H}} = p_{\text{OH}} - c^{\text{H}} (p_{\text{OH}} p_{\text{HN}})^f (p_{\text{OH}} - p_{\text{HN}}) - d^{\text{H}} (p_{\text{OH}} p_{\text{HN}})^g \quad (\text{S3})$$

$$p_{\text{HN}}^{\text{H}} = p_{\text{HN}} + c^{\text{H}} (p_{\text{OH}} p_{\text{HN}})^f (p_{\text{OH}} - p_{\text{HN}}) - d^{\text{H}} (p_{\text{OH}} p_{\text{HN}})^g \quad (\text{S4})$$

After a mathematically fitting the parameters d^{H} , c^{H} , f and g were slightly modified in comparison to our previous work (table S2).^{2,11}

Table S 2: Correction factors used for the hydrogen-bond correlations.

systems	f	g	c ^H	d ^H
weak and medium strong OHN bonds ¹¹	0	0	0	0
pyridine/HA and collidine/HA ¹¹ in CDF ₃ /CDF ₂ Cl	5	2	360	0.7
pyridine/HA and collidine/HA solid ¹³	5	2	360	0.7
imine/TRIP ²	8	2	360	0.3
imine/TiPSY, imine/TRIFP and imine/TRIM	7.3	1.36	349.9	0.33

In accordance with Limbach and Denisov, the measured NMR data of the hydrogen bonds were correlated with their geometries by using the concept of valence bond orders of Pauling.^{11,12,15} The valence bond orders for the hydrogen bonds of the proton and the heavy atoms within an OHN hydrogen bond are given by p_{OH}^H (equation S5) and p_{NH}^H (equation S6). Both values are dependent on the atom distances (r_{OH} and r_{NH}).

$$p_{OH}^H = \exp\left\{\frac{-(r_{OH} - r_{OH}^\circ)}{b_{OH}}\right\} \quad (S5)$$

$$p_{NH}^H = \exp\left\{\frac{-(r_{NH} - r_{NH}^\circ)}{b_{NH}}\right\} \quad (S6)$$

$$p_{OH}^H + p_{NH}^H = 1 \quad (S7)$$

3.2 Referencing of the ^{15}N chemical shift

As proposed in the literature, the ^{15}N chemical shifts were referenced to the chemical shift of the non-hydrogen bonded imine **11** ($\delta^{15}\text{N} = 340.8$ ppm, 300 K, CD_2Cl_2).¹² Thus, the ^{15}N chemical shifts reflect the deviation of the complexed imines from their neutral form ($\delta^{15}\text{N} = \sim 330$ ppm) and range from -90 to -150 ppm. Because of this correction $\delta(\text{N})^\circ$ can be set to 0.

3.3 Steiner-Limbach correlation curve: experimental ^1H and ^{15}N chemical shifts

Table S 3: NMR parameters ($\delta^1\text{H}$ and $\delta^{15}\text{N}$ chemical shift as well as $^1J_{\text{NH}}$) of $\text{HBF}_4/\text{imine}$, TRIP/imine, carboxylic acids and phenol/imine complexes in CD_2Cl_2 . All values are obtained from literature.²

Complex	$\delta^1\text{H}$ [ppm]	$\delta^{15}\text{N}$ [ppm]	$^1J_{\text{NH}}$ [Hz]	Solvent	T [K]	Ref.
$\text{HBF}_4/3E$	12.35	189.4	92.3	CD_2Cl_2	180	TMS
$\text{HBF}_4/3Z$	12.48	193.4	91.9	CD_2Cl_2	180	TMS
$\text{HBF}_4/5E$	12.23	182.8	92.5	CD_2Cl_2	180	TMS
$\text{HBF}_4/5Z$	12.26	188.2	92.6	CD_2Cl_2	180	TMS
R-TRIP/2E	17.68	224.3	75.4	CD_2Cl_2	180	TMS
R-TRIP/2Z	17.68	221.1	n.d.	CD_2Cl_2	180	TMS
R-TRIP/3E	17.07	216.0	79.2	CD_2Cl_2	180	CHDCl_2
R-TRIP/3Z	17.11	215.0	78.4	CD_2Cl_2	180	CHDCl_2
R-TRIP/4E	18.20	235.1	68.7	CD_2Cl_2	180	TMS
R-TRIP/4Z	18.20	228.0	74.8 ^[a]	CD_2Cl_2	180	TMS
R-TRIP/5E	16.47	206.6	82.2	CD_2Cl_2	180	TMS
R-TRIP/5Z	16.75	209.1	81.0	CD_2Cl_2	180	TMS
R-TRIP/6E	17.42	220.6	77.3	CD_2Cl_2	180	TMS
R-TRIP/6Z	17.42	217.9	n.d.	CD_2Cl_2	180	TMS
R-TRIP/10E	18.42	243.3	67.7	CD_2Cl_2	180	TMS
R-TRIP/10Z1	18.18	228.9	74.3	CD_2Cl_2	180	TMS
R-TRIP/10Z2	18.13	228.7	75.2	CD_2Cl_2	180	TMS
R-TRIP/11E	17.70	268.1	n.d.	CD_2Cl_2	180	TMS
R-TRIP/11Z	17.93	264.1	41.7	CD_2Cl_2	170	TMS
R-TRIP/11Z	18.85	240.6	60.6	CD_2Cl_2	180	TMS
R-TRIP/12	17.35	225.5	77.0	CD_2Cl_2	200	TMS
R-TRIP/13E	17.31	223.6	78.1	CD_2Cl_2	180	TMS
R-TRIP/13Z	17.07	221.7	79.3	CD_2Cl_2	180	TMS
4-NO ₂ -Phenol/3	13.43	299.3	n.d.	$\text{CDCl}_2\text{F}^{[b]}$	130	TMS
4-Cl-Phenol /5	11.81	299.7	n.d.	$\text{CDCl}_2\text{F}^{[b]}$	130	TMS
3,5-Cl-Phenol/5	12.25	297.1	n.d.	$\text{CDCl}_2\text{F}^{[b]}$	130	TMS
3-CF ₃ -Phenol/5	11.96	299.0	n.d.	$\text{CDCl}_2\text{F}^{[b]}$	130	TMS
Acetic Acid/5	14.60	294.3	n.d.	$\text{CDCl}_2\text{F}^{[b]}$	130	TMS
TMA/5	14.34	295.8	n.d.	$\text{CDCl}_2\text{F}^{[b]}$	130	TMS

^[a]derived from HN-HMBC ^[b] Freonic mixture; $\text{CDCl}_2\text{F}/\text{CDClF}_2$ ratio slightly varies between samples. For sample preparation, see reference.²

Table S 4: NMR parameters ($\delta^1\text{H}$ and $\delta^{15}\text{N}$ chemical shift as well as $^1J_{\text{NH}}$) of TRIFP/imine, TiPSY/imine and TRIM/imine complexes in CD_2Cl_2 .

Complex	$\delta^1\text{H}$ [ppm]	$\delta^{15}\text{N}$ [ppm]	$^1J_{\text{NH}}$ [Hz]	Solvent	T [K]	Ref.
R-TRIFP/2E	16.49	210.6	82.8	CD_2Cl_2	170	TMS
R-TRIFP/2Z	16.96	215.2	81.1	CD_2Cl_2	170	TMS
R-TRIFP/3E	15.95	204.2	85.1	CD_2Cl_2	170	TMS
R-TRIFP/3Z	16.50	209.9	82.7	CD_2Cl_2	170	TMS
R-TRIFP/4E	17.09	218.2	80.8	CD_2Cl_2	170	TMS
R-TRIFP/4Z	17.39	220.4	80.5	CD_2Cl_2	170	TMS
R-TRIFP/5E	15.39	196.4	86.0	CD_2Cl_2	170	TMS
R-TRIFP/5Z	16.11	204.4	85.1	CD_2Cl_2	170	TMS
R-TRIFP/6E	16.18	207.1	83.0	CD_2Cl_2	170	TMS
R-TRIFP/6Z	16.79	213.1	82.3	CD_2Cl_2	170	TMS
R-TiPSY/2E*	16.79	219.6	77.3	CD_2Cl_2	180	TMS
R-TiPSY/2Z*	17.16	222.7	73.9	CD_2Cl_2	180	TMS
R-TiPSY/3E	16.12	211.3	81.2	CD_2Cl_2	180	TMS
R-TiPSY/3Z	16.64	216.6	78.1	CD_2Cl_2	180	TMS
R-TiPSY/4E	17.32	228.3	73.1	CD_2Cl_2	180	TMS
R-TiPSY/4Z	17.56	228.3	71.8	CD_2Cl_2	180	TMS
R-TiPSY/5E	15.53	203.6	83.7	CD_2Cl_2	180	TMS
R-TiPSY/5Z	16.24	211.3	80.0	CD_2Cl_2	180	TMS
R-TiPSY/6E	16.50	216.3	79.2	CD_2Cl_2	180	TMS
R-TiPSY/6Z	17.00	220.6	76.0	CD_2Cl_2	180	TMS
R-TiPSY/7E	16.30	212.0	81.4	CD_2Cl_2	180	TMS
R-TiPSY/7Z	16.90	218.8	77.2	CD_2Cl_2	180	TMS
R-TiPSY/8E	15.78	207.8	83.5	CD_2Cl_2	180	TMS
R-TiPSY/8Z	16.74	218.3	77.0	CD_2Cl_2	180	TMS
R-TiPSY/9E	16.13	212.0	81.7	CD_2Cl_2	180	TMS
R-TiPSY/9Z	16.60	218.8	77.7	CD_2Cl_2	180	TMS
R-TRIM/3E	16.26	208.0	83.9	CD_2Cl_2	180	TMS
R-TRIM/3Z	16.72	211.5	80.9	CD_2Cl_2	180	TMS
R-TRIM/4E	17.51	224.6	77.3	CD_2Cl_2	180	TMS
R-TRIM/4Z	17.76	224.1	76.0	CD_2Cl_2	180	TMS
R-TRIM/5E	15.80	200.5	85.4	CD_2Cl_2	180	TMS
R-TRIM/5Z	16.31	206.0	82.2	CD_2Cl_2	180	TMS

*this complex showed precipitation inside the NMR tube

3.4 Plot of $^1J_{\text{HN}}$ against δ_{OHN}

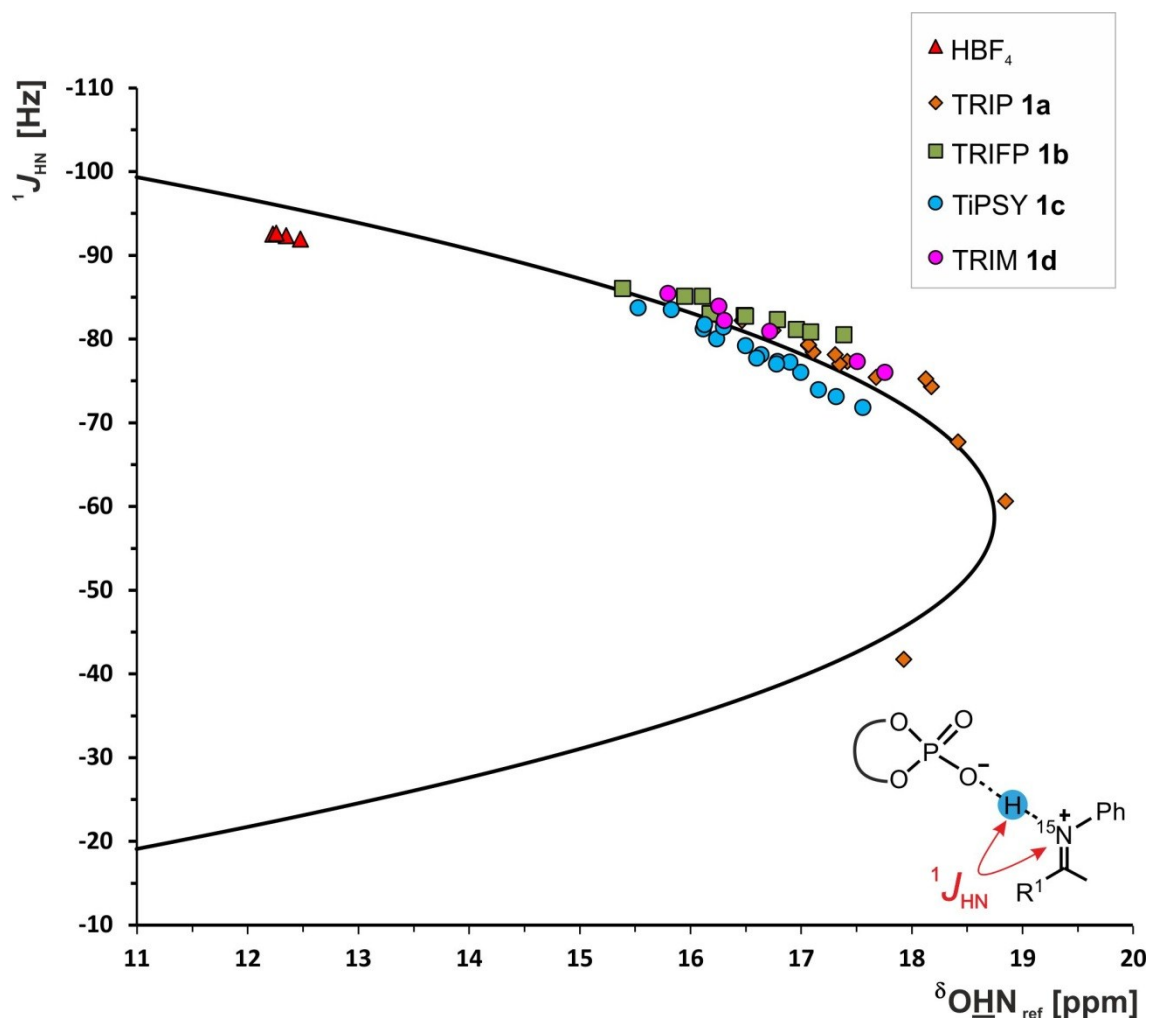


Figure S 1: Plot of $^1J_{\text{HN}}$ values against $\delta(\text{OHN})$. Experimental $\delta(\text{OHN})/ ^1J_{\text{HN}}$ pair values derived from TiPSY/imine complexes (blue), TRIFP/imine complexes (green), TRIM/imine (pink), TRIP/imine complexes² (orange) and $\text{HBF}_4/\text{imine}^2$ (red).

Measurements of scalar couplings $^1J_{\text{NH}}$ in CPA/imine complexes were also performed. Also, the ^1H chemical shift and scalar coupling are related to one another according to the following equation S10:^{11,12}

$$^1J(\text{OHN}) = ^1J(\text{HN})^{\circ} p_{\text{HN}^{\text{H}}} - 8^1J(\text{OHN})^* (p_{\text{OH}^{\text{H}}})^2 p_{\text{HN}^{\text{H}}} \quad (\text{S10})$$

Three clusters appeared corresponding to each of the four investigated catalysts. The complexes formed with TRIP have overall higher ^1H chemical shift values (~16.5 ppm to ~18.5 ppm) compared to the complexes formed with TiPSY, TRIM, and TRIFP. This indicates the formation of a stronger hydrogen bond. Differences in ^1H chemical shifts between the other three catalysts are smaller. Still, higher ^1H shift values were found for complexes involving TiPSY and TRIM compared to the TRIFP/imine-complexes.

On the other hand, the separation between TiPSY, TRIM and TRIFP clusters is mainly due to the $^1J_{\text{NH}}$ values (for values see table S3 and S4). Consistently higher $^1J_{\text{NH}}$ values (smaller in absolute values) were obtained with TiPSY complexes followed by TRIM and TRIFP. Since the focus of the curve (right side of the plot) corresponds to the shorter hydrogen bonds, complexes formed with TiPSY are overall slightly stronger than complexes formed with TRIM and TRIFP.

3.5 Plot of $^1J_{\text{HN}}$ against δ_{OHN}

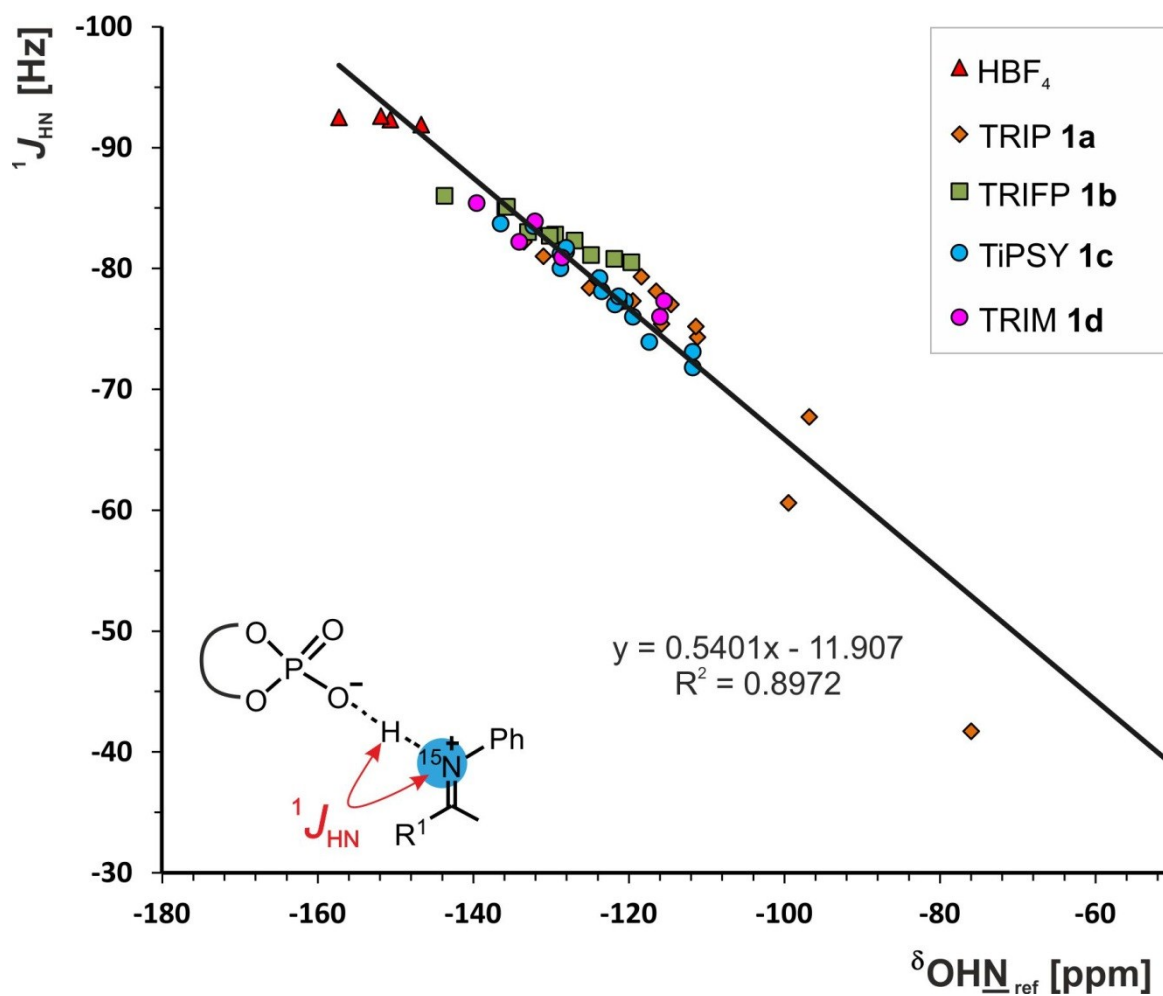


Figure S 2: Plot of $^1J_{\text{HN}}$ values against δ_{OHN} . Experimental $\delta_{\text{OHN}}/^1J_{\text{HN}}$ pairs derived from TiPSY/imine complexes (blue), TRIFP/imine complexes (green), TRIM/imine (pink), TRIP/imine complexes² (orange) and HBF₄/imine² (red). δ_{OHN} was referenced to 11 (340 ppm, 300K).

3.6 Enlarged section of the Steiner-Limbach curve

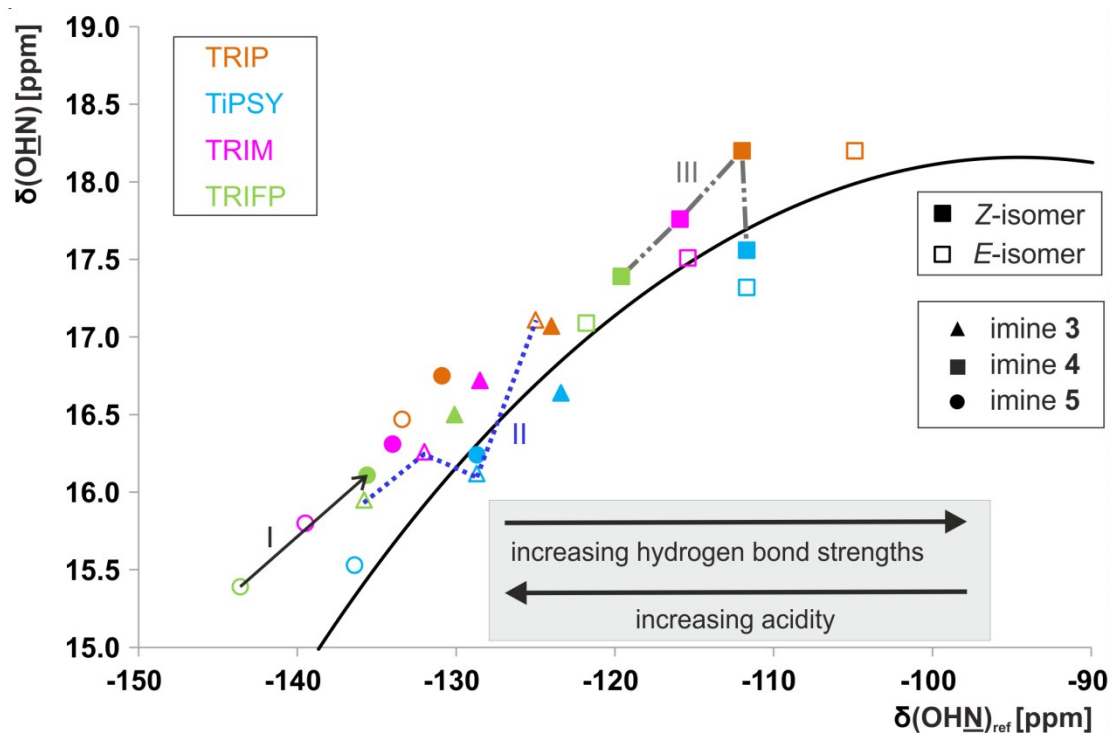


Figure S 3: Enlarged section of the Steiner-Limbach curve showing only the binary complexes of CPAs **1a-1d** and imines **3, 4** and **5**. The arrow I visualizes the observed increasing hydrogen bond strengths for the Z-complexes. The comparison of the hydrogen bond strengths of the different CPAs with one given imine is illustrated with the dotted lines II (E-complexes) and III (Z-complexes). These trends are exemplary shown with one imine but can be observed for imines **3-5**.

4 Comparison of the calculated and experimental $^1J_{\text{NH}}$

Table S 5: Experimental and calculated $^1J_{\text{NH}}$ coupling constants for all catalysts with imines 3, 4 and 5 are shown. The experimental values are obtained in CD_2Cl_2 at 180K.

catalyst	imine	$^1J_{\text{NH}}$ [Hz] calc	$^1J_{\text{NH}}$ [Hz] exp
TRIP	3E	-79.87	79.2
	3Z	-77.24	78.4
	4E	-77.35	68.7
	4Z	-75.04	74.8
	5E	-82.03	82.2
	5Z	-79.42	81.0
TRIFP	3E	-81.76	85.1
	3Z	-82.08	82.7
	4E	-79.65	80.8
	4Z	-80.80	80.5
	5E	-82.86	86.0
	5Z	-83.56	85.1
TIPSY	3E	-80.42	81.2
	3Z	-78.59	78.1
	4E	-76.41	73.1
	4Z	-76.00	71.8
	5E	-81.84	83.7
	5Z	-80.49	80.0
TRIM	3E	-81.65	83.9
	3Z	-78.74	80.9
	4E	-78.82	77.3
	4Z	-76.13	76.0
	5E	-83.63	85.4
	5Z	-80.25	82.2

5 Plots of $^1J_{\text{NH}}$ vs. Hammett σ_{para} constants for *E*- and *Z*-complexes

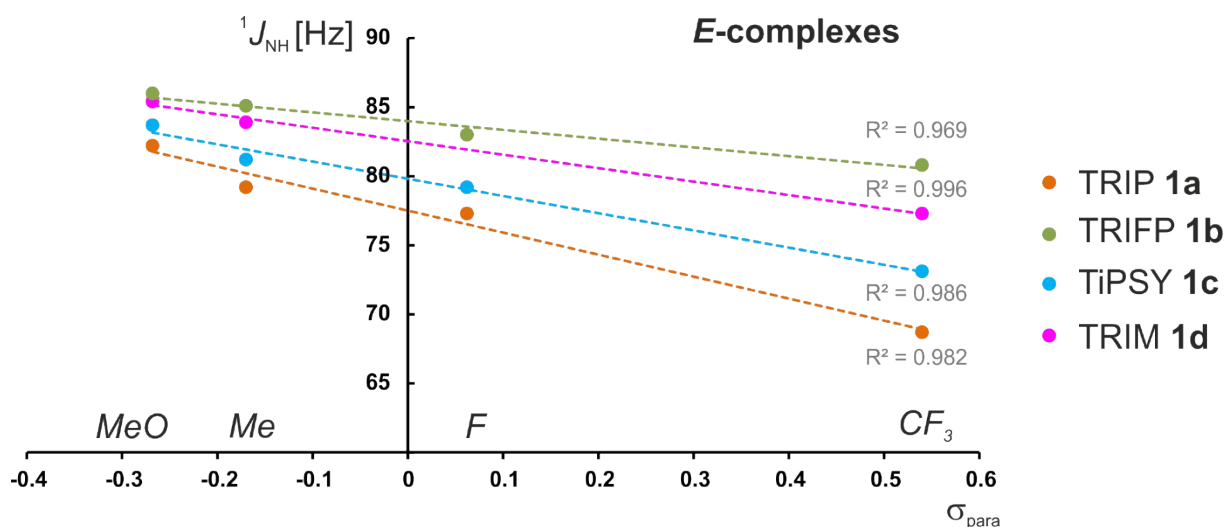


Figure S 4: Plot of experimental $^1J_{\text{HN}}$ values against Hammett σ_{para} constants for the *E*-complexes of phosphoric acids **1a** – **1d** with imines **3** – **6**. Data are plotted for TiPSY/imine complexes (blue), TRIFP/imine complexes (green), TRIM/imine (pink), and TRIP/imine complexes (orange).

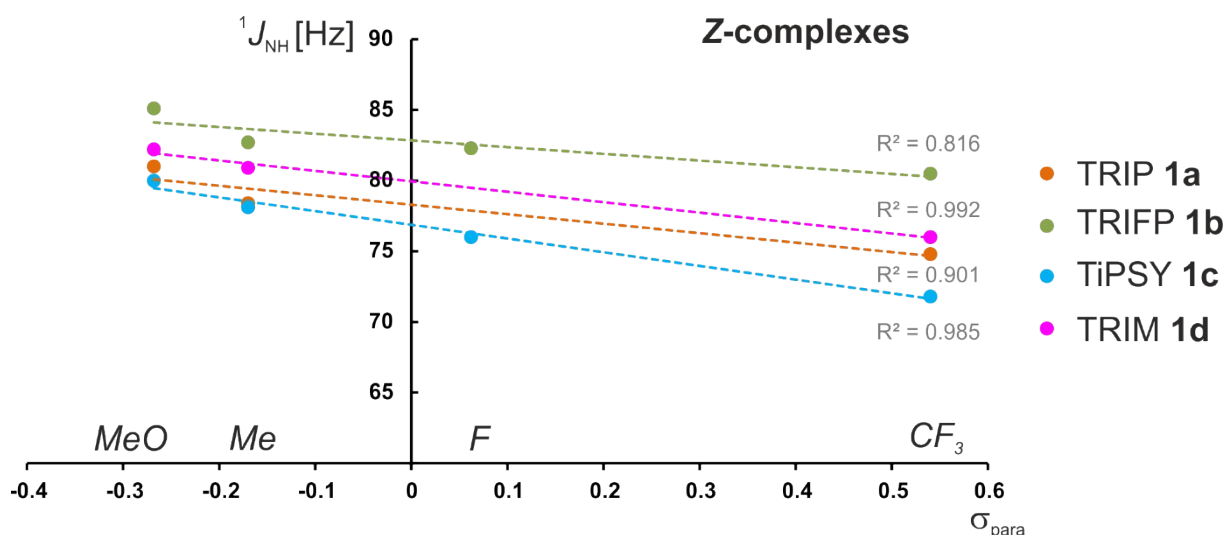


Figure S 5: Plot of experimental $^1J_{\text{HN}}$ values against Hammett σ_{para} constants for the *Z*-complexes of phosphoric acids **1a** – **1d** with imines **3** – **6**. Data are plotted for TiPSY/imine complexes (blue), TRIFP/imine complexes (green), TRIM/imine (pink), and TRIP/imine complexes (orange).

6 Calculation of the external pKa values

An experimental acidity scale with pK_a values of different Brønsted acid catalysts, including TRIP and TRIFP was published by O'Donoghue in 2011.¹⁶ To our knowledge, there is no such scale including the four catalysts TRIP, TRIFP, TRIM and TiPSY. Therefore, relative pK_a values in DCM of TRIP, TRIFP, TRIM and TiPSY for an external acidity scale were calculated at DG₁₈₀ SCS-MP2/CBS//TPSS-D3/def2-SVP level of theory using equation S11 and S12.

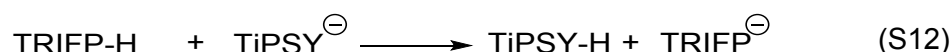
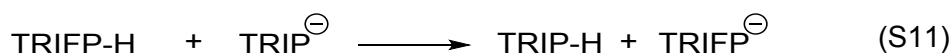


Table S 6: Calculated relative (in DCM at 180K) and experimental (in DMSO at 25°C)¹⁶ pK_a values of the CPAs.

	pK _a _{calc}	pK _a _{exp}
TRIFP	0	0
TRIP	+0.85	+1.59
TiPSY	+6.00	n.a.
TRIM	+1.57	n.a.

The calculations show the lowest pK_a value for TRIFP followed by TRIP, TRIM and TiPSY. The trend of the external acidity (pK_a_{TRIFP} < pK_a_{TRIP} < pK_a_{TRIM} < pK_a_{TiPSY}) predicted in the calculations does not correlate with the internal acidity scale obtained from the Steiner-Limbach analysis (*E*-imines: pK_a_{TRIFP} < pK_a_{TRIM} < pK_a_{TiPSY} < pK_a_{TRIP}; *Z*-imines: pK_a_{TRIFP} < pK_a_{TRIM} < pK_a_{TRIP} < pK_a_{TiPSY}). This demonstrates that other interactions (dispersion, steric, and electrostatic) significantly contribute in the internal scale.

7 Reaction kinetics of the transfer hydrogenation

7.1 Procedure for the *in-situ* kinetics

The reactions were performed with a 0.1 molar solution of imine **3** or **5** with 1.4 equivalents of diethyl 1,4-dihydro-2,6-dimethyl-3,5-pyridinedicarboxylate and 1 mol% of catalysts (TRIFP, TRIM and TiPSY) at 313.15 K in 0.5 ml deuterated dichloromethane. Due to solubility reasons, the reaction with TRIM was done in a 0.065 molar solution of **3** with 1.4 equivalents of diethyl 1,4-dihydro-2,6-dimethyl-3,5-pyridinedicarboxylate and 1 mol% of catalysts at 313.15 K in 0.5 ml deuterated dichloromethane. The imines were prepared as described in the experimental section 1.2. Both catalysts and Hantzsch ester were purchased from Sigma Aldrich. To compare the intensities of the spectra, the intensity of the alpha-methyl group of the imine in the first spectrum was used to calibrate the intensities of the alpha-methyl groups of the products. For this reaction in toluene higher yields and enantiomeric excesses are reported. Since structure determination¹⁷ and hydrogen bond analysis were done in dichloromethane, this solvent was also used for the reaction kinetics. Additionally, the signals in dichloromethane are better separated and enable therefore a more exact integration.

The fastest reaction is observed with TRIP, followed by TRIM and TRIFP. Catalyst TiPSY shows only a slow product formation.

7.2 Procedure for the *ex-situ* kinetics

A Schlenk tube with an attached septum was dried at 350 °C for 5 min under reduced pressure and then cooled down to room temperature. Imine **5** (73.7 mg, 327 μmol, 1.0 eq.) and Hantzsch Ester (116.0 mg, 457.8 μmol, 1.4 eq.) were weighed into the tube. The tube was evacuated and flushed with argon three times. A standard stock solution of 1,3,5-trimethoxybenzene (54 mM) in anhydrous toluene was prepared and 3 mL of the standard-stock solution were added to the tube under argon flow. The setup was placed into a metal-heating block and preheated to 35 °C. A catalyst stock solution was prepared by dissolving the catalyst (2.9 mM) in anhydrous toluene. To start the reaction, the catalyst stock solution (1.0 mL, 0.009 eq catalyst) was added to the reaction mixture. After 1, 5, 10, 15, 20, 25, 30, 45 and 60 min, samples of the reaction mixture (≈ 0.1 mL) were taken via a septum and quenched by adding to a solution of n-hexane (2.0 mL) and NEt₃ (10 μL, 7.3 μg, 0.072 mmol, 100 eq. based on the catalyst). The mixture was filtered through a syringe filter and analyzed by CSP-HPLC. It was shown that the addition of NEt₃ quenches the reaction and that the standard does not interfere with the reaction.

HPLC conditions: CSP-HPLC, CHIRAPACK IC column (4.6mm x 250 mmL, particle size: 5 μm), eluent n-hexane/*i*-propanol 99/1, flowrate 0.9mL/min, column compartment temperature 20°C, λ = 220 nm. retention times: toluene/NEt₃: τ₁ = 3.73 min; major (*R*)-amine: τ₂ = 10.1 min; minor (*S*)-amine: τ₃ = 11.1 min; 1,3,5-trimethoxybenzene: τ₄ = 15.4 min; imine **5**: τ₅ = 24.9 min; HE-pyridin: τ₆ = 42.8 min;

7.3 Kinetics of the transfer hydrogenation with imine **5**

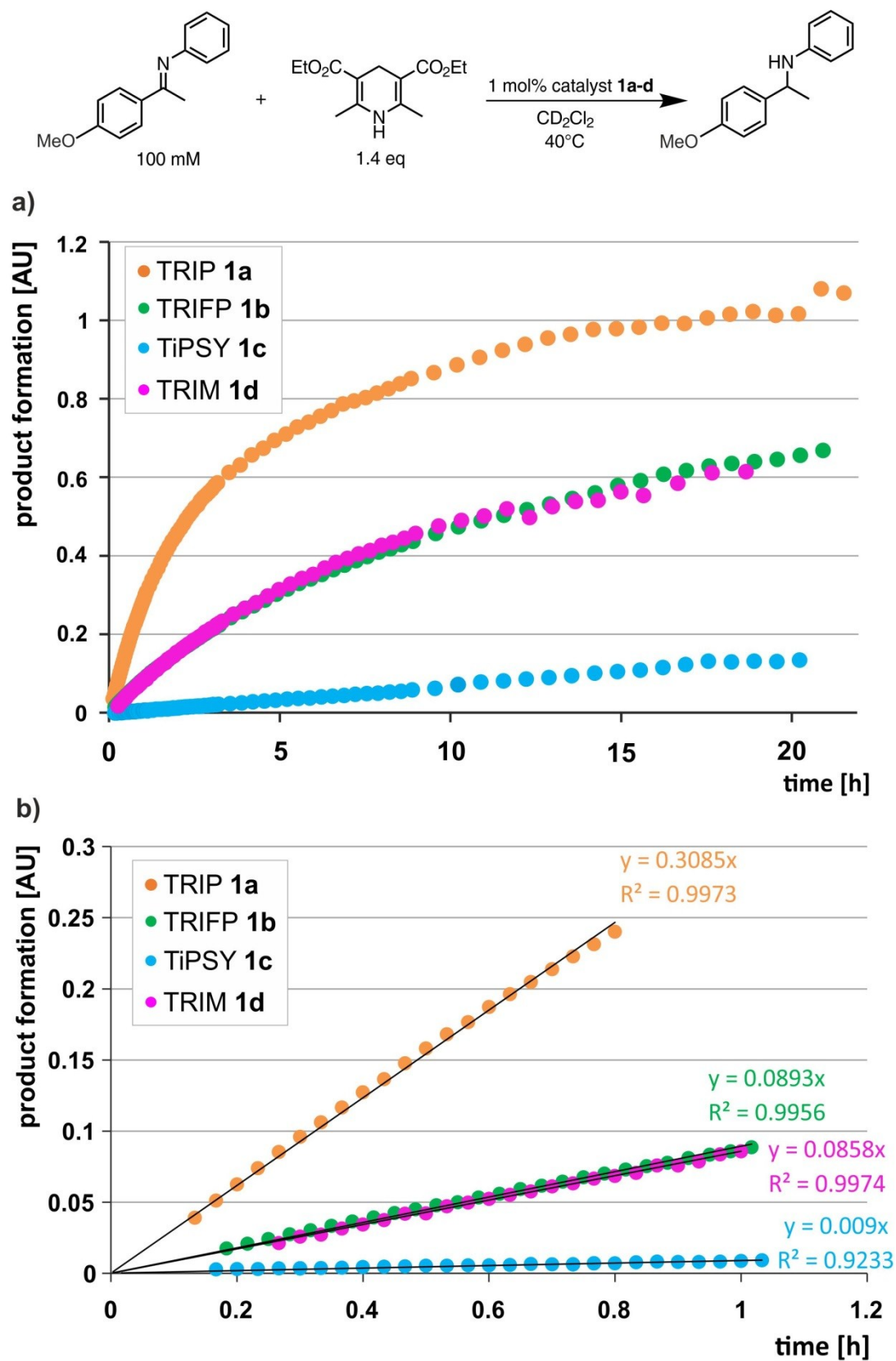


Figure S 6: a) The reaction profiles for the symmetric transfer hydrogenation of imine **5** are shown. The kinetics were done in-situ in the NMR spectrometer with 1.4 equivalents of Hantzsch ester and 1 mol% catalyst (TRIP, TRIFP, TiPSY and TRIM) at 40°C in CD₂Cl₂ b) the linear ranges enable the access to the rate constants.

In general, the reaction with imine **5** is significantly slower than with imine **3**. For all catalysts, the reaction rate of the transfer hydrogenation is reduced to more than half. This is also reflected in the isolated yields after five hours.¹⁸

Also with imine **5** we identified TRIP as the most reactive catalyst and the reaction catalyzed by TiPSY is by far the slowest. However, the reactivity of TRIM and TRIFP is more or less the same (see Figure S4). These kinetic profiles were recorded in-situ in the NMR-spectrometer. The lower reactivity of TRIM with imine **5** compared to imine **3** may also be due to the low solubility of TRIM in CD₂Cl₂. Thus, following the reaction kinetics without stirring has some potential drawbacks. Less amount of catalyst is dissolved in the reaction mixture and the reaction rate is slowed down compared to the other well-soluble catalysts. For this reason, ex-situ kinetics under the normal reaction conditions (in toluene at 35°C) were done. Here we observed the same result as with imine **3**: the reaction with TRIP is the fastest, followed by TRIM and TRIFP. The amount of product for the reaction catalyzed by TiPSY is small and could not be detected by HPLC.

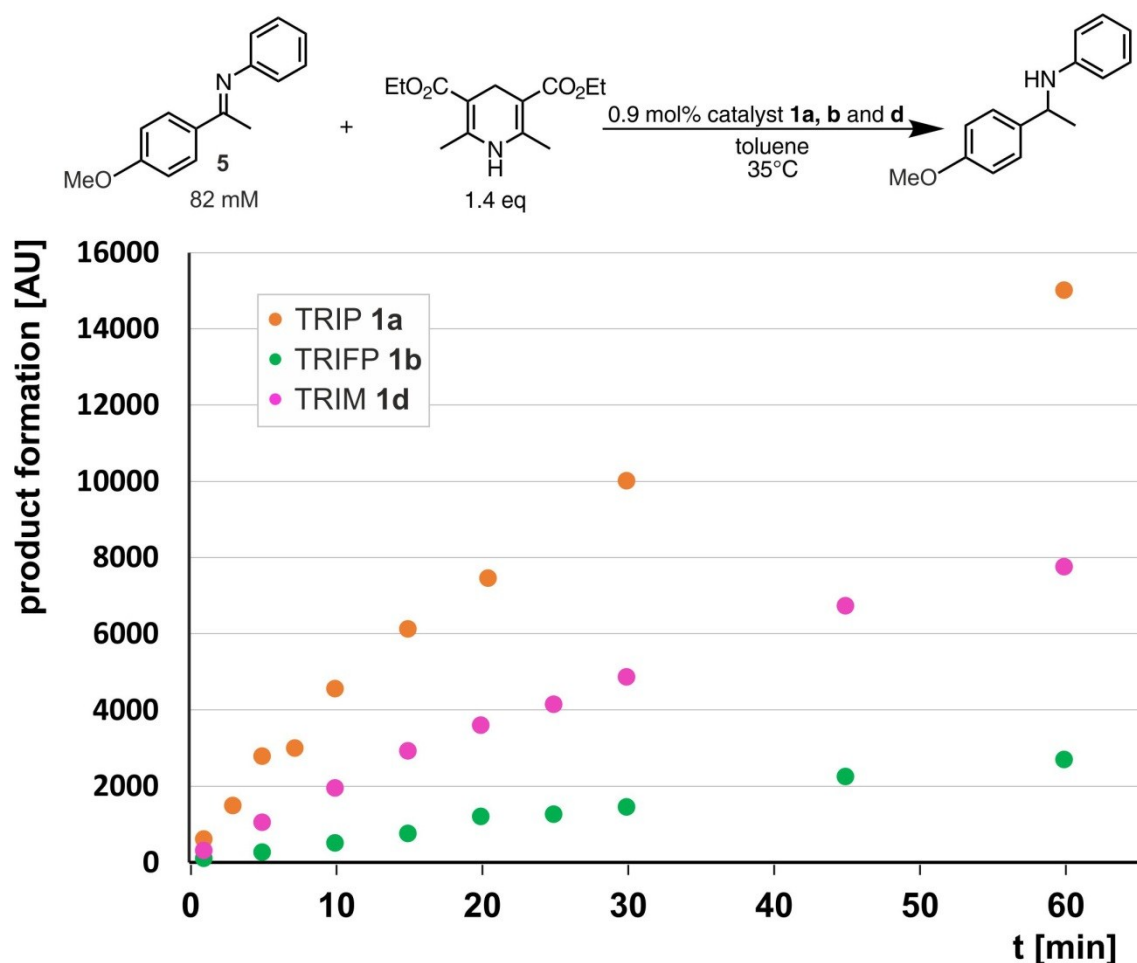
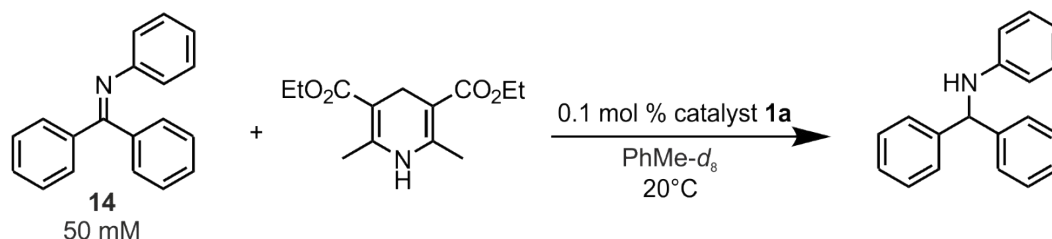


Figure S 7: The linear ranges of the reaction profiles for the asymmetric transfer hydrogenation of imine **5** are shown. The kinetics were done ex-situ with 1.4 equivalents of Hantzsch ester and 0.9 mol% catalyst (TRIP, TRIFP, TiPSY and TRM) at 35°C in toluene. The amount of product was analyzed with chiral HPLC.

7.4 Procedure for the in-situ kinetics of a non-isomerizable imine reaction



The following kinetic experiments were conducted to show the dependence of the reaction rate on the dissolved Hantzsch ester concentration, without any interference from the isomerization process and the undissolved Hantzsch ester. The loading of the catalyst was set to 0.1 mol % due to the high reactivity of *N*,1,1-triphenylmethanimine (**14**) under the standard conditions (0.9 mol % catalyst, 35°C).

Sample A: Into an NMR tube charged with *N*,1,1-triphenylmethanimine (9.0 mg, $35\ \mu\text{mol}$) was added a solution of **1a** ($0.23\ \mu\text{M}$ solution in $\text{PhMe-}d_8$, 0.15 mL, $0.035\ \mu\text{mol}$, 0.1 mol %). In a separate flask, $\text{PhMe-}d_8$ (1.3 mL) was added to Hantzsch ester (29.0 mg, 0.11 mmol) and 1,3,5-trimethoxybenzene (2.88 mg, 0.017 mmol). The heterogenous mixture was stirred at rt for 15 min and then an aliquot (0.55 mL) was taken up by a syringe and filtered *via* a syringe filter into the NMR tube containing the imine and the catalyst to achieve the total volume of 0.7 mL. The homogenous sample was shaken thoroughly, inserted into a 600 MHz spectrometer, equilibrated at 293.15 K, and the kinetic profile was recorded.

Sample B: To achieve a different concentration of the dissolved Hantzsch ester, the imine/**1a** mixture was prepared as previously, and diluted by additional solvent (0.3 mL). Hantzsch ester mixture (0.25 mL) was then filtered into the NMR tube. The kinetic profile was recorded as previously stated. In contrast, directly diluting the Hantzsch ester mixture led to the same final Hantzsch ester concentration, as more ester readily dissolved.

Sample A: imine/standard/(Hantzsch ester+Hantzsch pyridine) ratio of 5.8:1:0.5.

Sample B: imine/standard/(Hantzsch ester+Hantzsch pyridine) ratio of 12.2:1:0.5.

Product *N*-benzhydrylaniline: ^1H NMR (600 MHz, $\text{PhMe-}d_8$, 293.15 K): δ 7.22 – 7.18 (m, 4H), 7.13 – 7.09 (m, 4H), 7.07 – 7.03 (m, 4H), 6.70 (tt, $J = 7.4, 1.0$ Hz, 1H), 6.42 – 6.38 (m, 2H), 5.38 (d, $J = 4.1$ Hz, 1H), 3.87 (br d, $J = 4.0$ Hz, 1H).

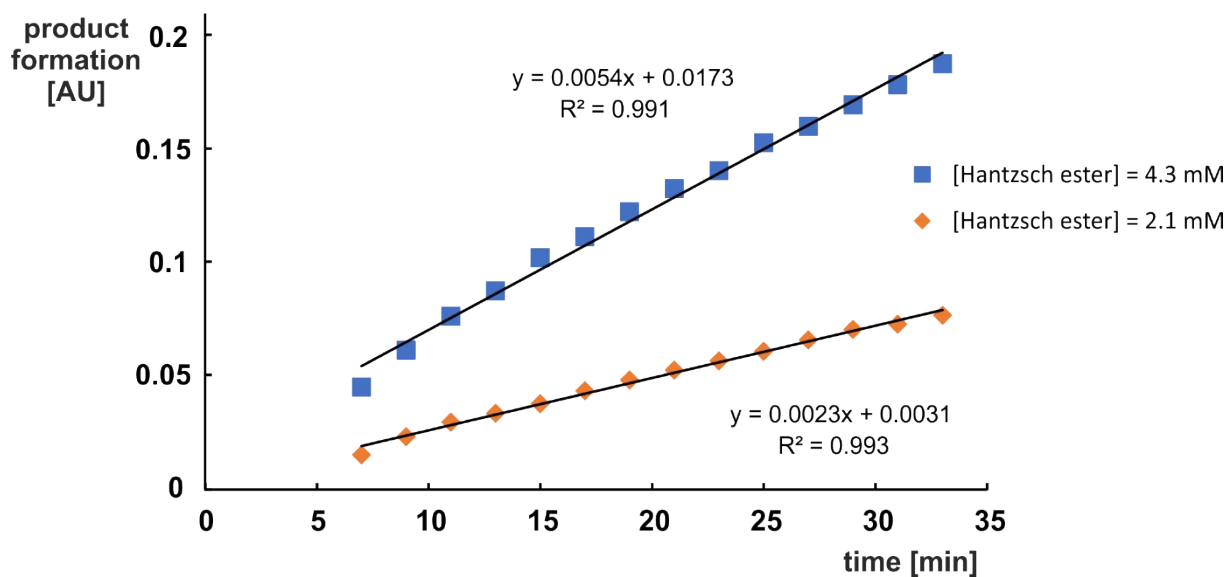


Figure S 8: The linear range of the reaction profiles for the transfer hydrogenation of non-isomerizable imine **14** are shown. The kinetics were done in-situ with dissolved Hantzsch ester and 0.1 mol% catalyst (TRIP) at 20°C in PhMe- d_8 . The amount of product was analyzed by integration of the ^1H spectra.

The ratio of the Hantzsch ester concentrations is 2.10:1 and the ratio of the initial relative rates is 2.35:1 in these experiments, suggesting a first-order reaction with respect to the Hantzsch ester.

8 Amount of free imine in the ^1H spectra

The amount of free imine is experimentally accessible by the integration of the ^1H -signals obtaining from the OMe-groups of imine **5** in 1:1 sample of the catalyst and imine **5** in CD_2Cl_2 at 180K. In this region three different signals (free imine, hydrogen bonded *E*- and *Z*-imine) are visible. For referencing the signal of the hydrogen-bonded *E*-imine was set to 1 in all cases. The determination of the amount of free imine for other imines is unreliable because of signal overlapping.

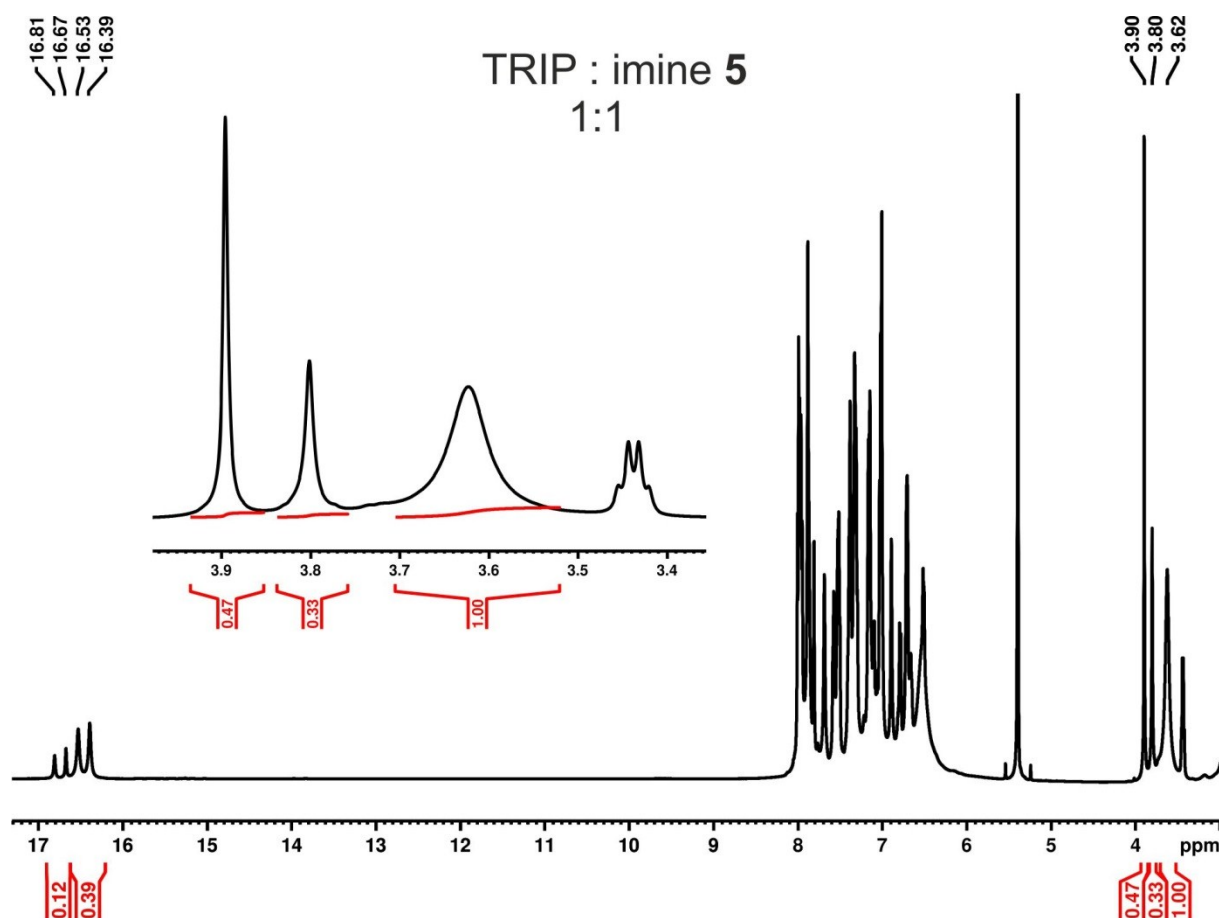


Figure S 9: ^1H -spectra of a 1:1 sample of TRIP and imine **5** in CD_2Cl_2 at 180K. For the determination of the amount of free imine the signals of the OMe-groups (free imine: 3.90 ppm, *Z*-imine: 3.80 ppm and *E*-imine: 3.62 ppm) were used. Furthermore, the signals of the hydrogen-bonded protons (*Z*-imine: 16.75 ppm and *E*-imine: 16.47 ppm) are shown.

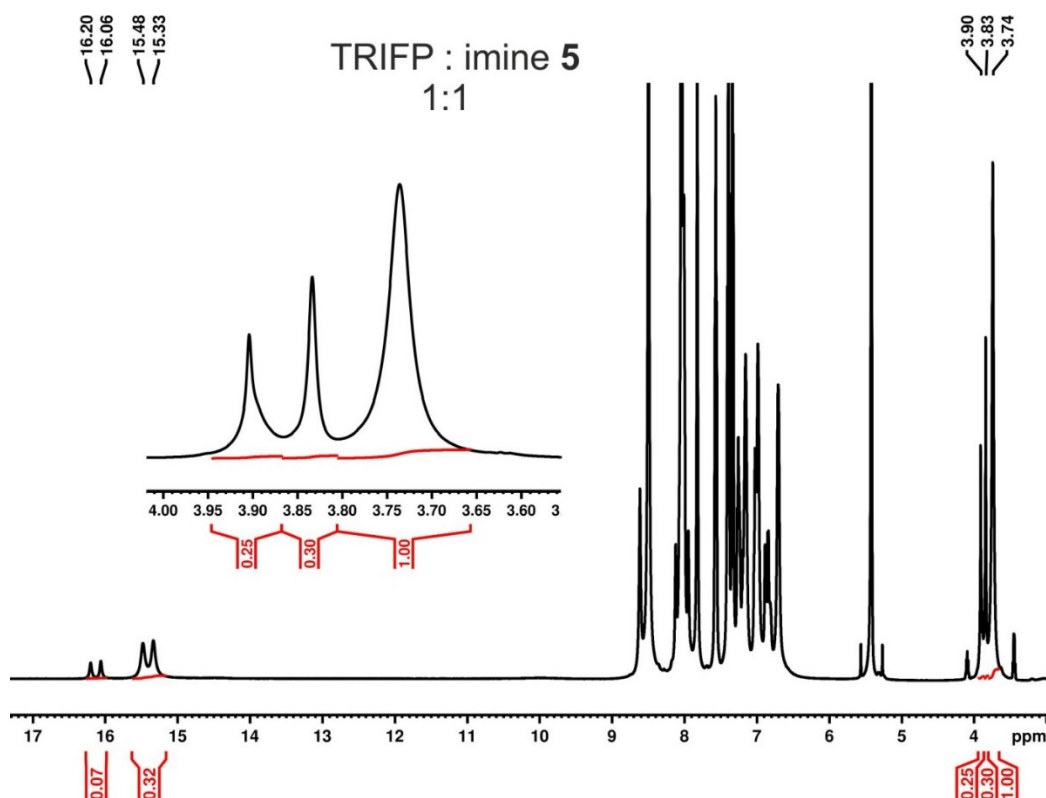


Figure S 10: ^1H -spectra of a 1:1 sample of TRIFP and imine **5** in CD_2Cl_2 at 180K. For the determination of the amount of free imine the signals of the OMe-groups (free imine: 3.90 ppm, *Z*-imine: 3.83 ppm and *E*-imine: 3.74 ppm) were used. Furthermore, the signals of the hydrogen-bonded protons (*Z*-imine: 16.11 ppm and *E*-imine: 15.39 ppm) are shown.

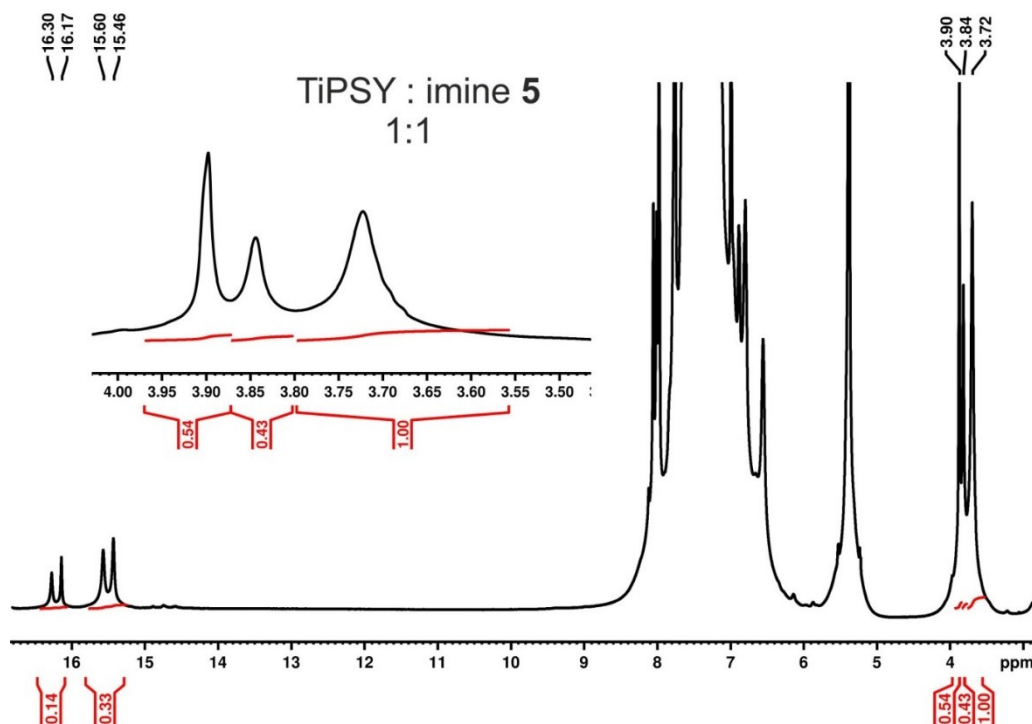


Figure S 11: ^1H -spectra of a 1:1 sample of TiPSY and imine **5** in CD_2Cl_2 at 180K. For the determination of the amount of free imine the signals of the OMe-groups (free imine: 3.90 ppm, *Z*-imine: 3.84 ppm and *E*-imine: 3.72 ppm) were used. Furthermore, the signals of the hydrogen-bonded protons (*Z*-imine: 16.24 ppm and *E*-imine: 15.53 ppm) are shown.

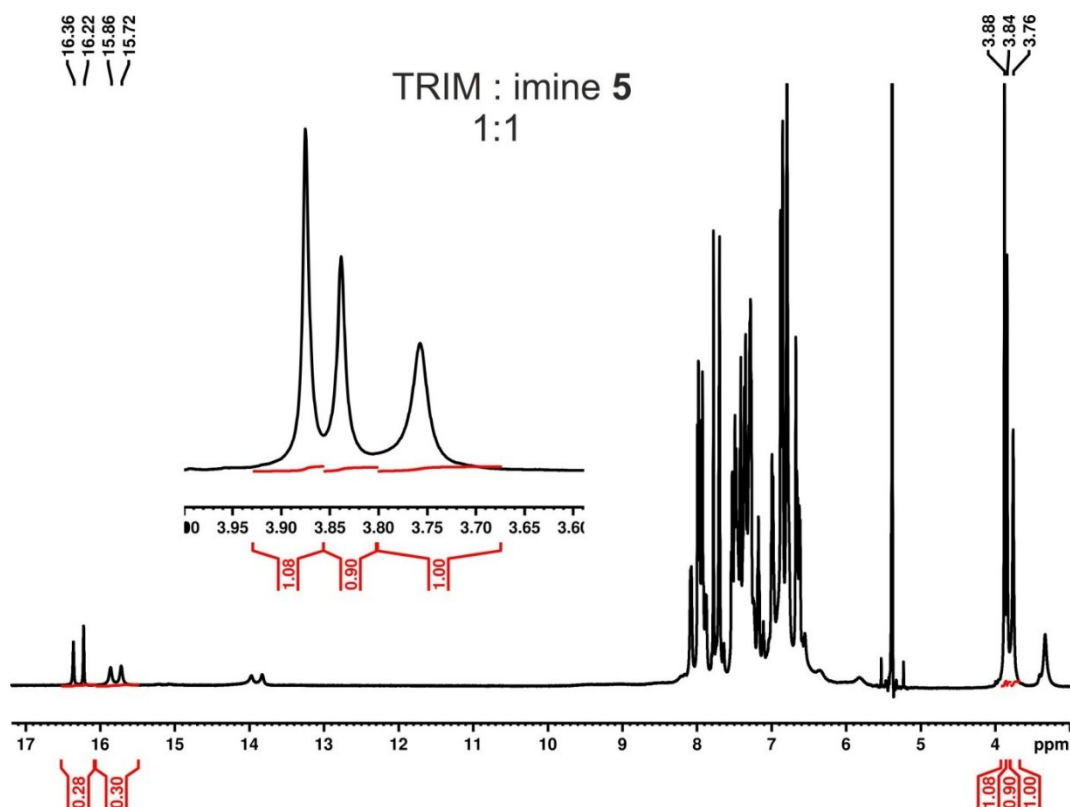


Figure S 12: ^1H -spectra of a 1:1 sample of TRIM and imine **5** in CD_2Cl_2 at 180K. For the determination of the amount of free imine the signals of the OMe-groups (free imine: 3.88 ppm, Z-imine: 3.84 ppm and E-imine: 3.76 ppm) were used. Furthermore, the signals of the hydrogen-bonded protons (Z-imine: 16.31 ppm and E-imine: 15.80 ppm) are shown.

For all cases, the obtained integrals (of free imine as well as hydrogen bonded E- and Z-imine) and the amount of free imine **5** are summarized in Table S9. Binary complex association constants were calculated from the equilibrium as $K_a = [\text{binary complex}] / ([\text{free imine}] [\text{free CPA}]) = c_0(1-\alpha)/(c_0\alpha)^2$, with $c_0 = 0.050$ M and α is the % amount of the free imine.

Table S 7: The integrals of the ^1H -signals in CD_2Cl_2 at 180 K are summarized. The OMe signals for the free imine as well as the hydrogen bonded E- and Z-imines were integrated and the the amount of free imine was calculated.

catalyst	imine	integral (E)	integral (Z)	integral (free)	free [%]	K_a [M^{-1}]
TRIP	5	1	0.31	0.47	26	219
TRIFP	5	1	0.30	0.25	16	656
TiPSY	5	1	0.43	0.54	27	200
TRIM	5	1	0.90	1.08	36	106

9 Formation of the binary complex

TRIM/5 180 K
blue: t = 7 min
red: t = 3 d

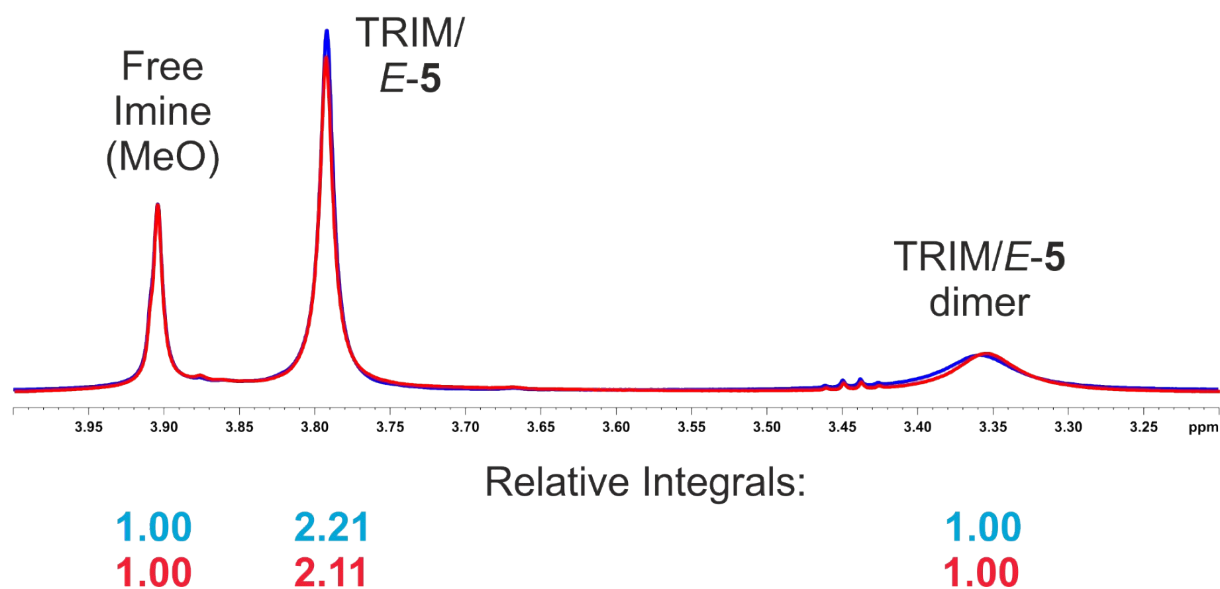


Figure S13: Fast formation of the binary complex. The blue spectrum was recorded 7 min after solvation of TRIM and imine **5** at -80°C , the red spectrum 3 days afterward (the sample was continuously kept at -80°C). The relative integrals show, that no further complexation occurs after 7 min.

10 Reactivity at 180 K and 220 K of TRIM/imine complex with Hantzsch Ester

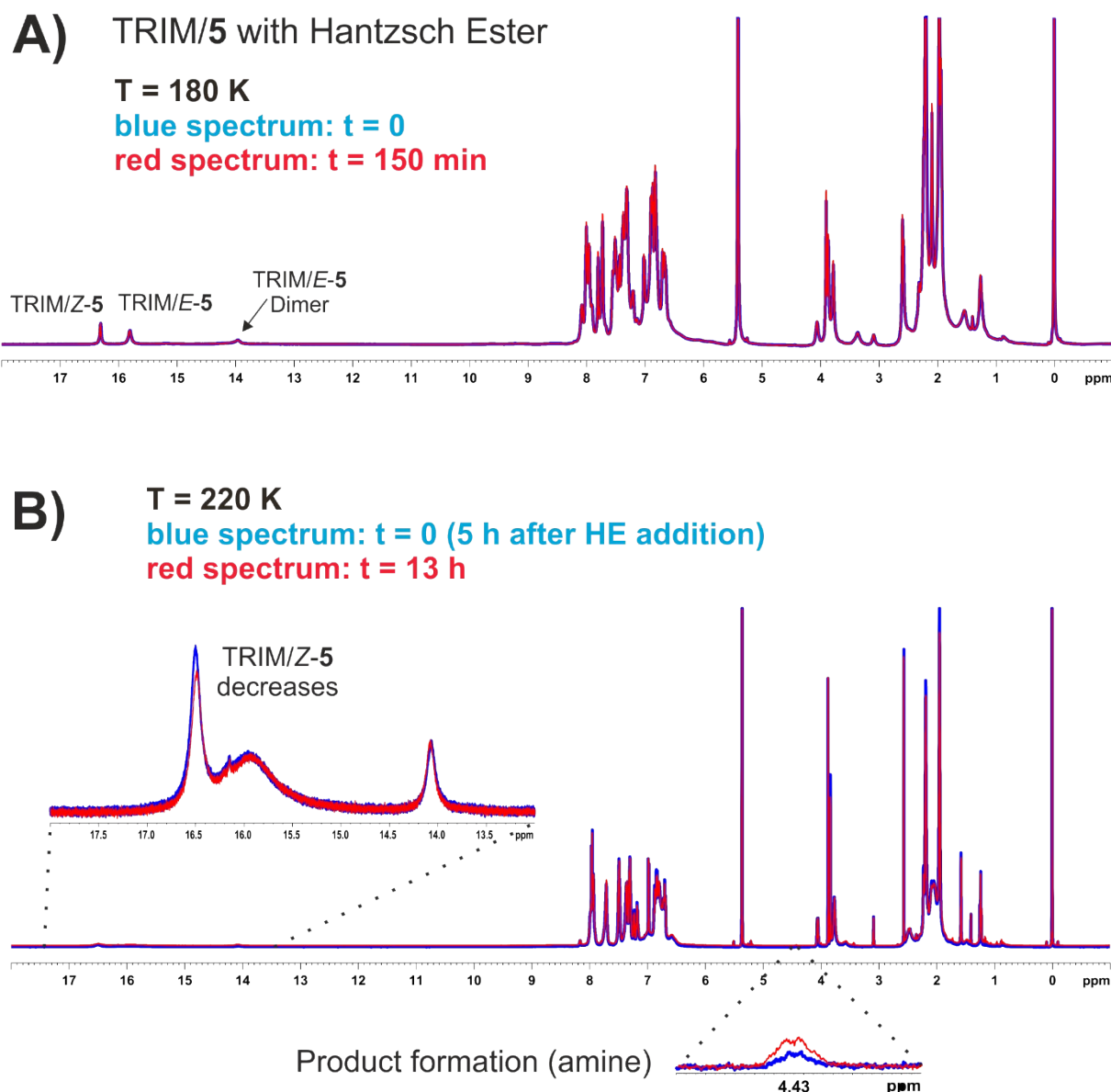


Figure S14: A 1:1 sample of TRIM and imine **5** was prepared (50 mM) at room temperature. The sample was cooled to 180 K and Hantzsch Ester (1.4 eq.) was added. **A)** Shows two overlapped spectra of the sample (blue: directly after HE addition, red: 150 min after the blue spectrum). Both spectra are identical despite the presence of dissolved Hantzsch Ester and binary *E*- and *Z*-complex, showing that no reaction occurs at 180 K. **B)** Overlap of two spectra of the sample ($\Delta t = 13$ h) at 220 K. The blue spectrum ($t=0$) was recorded 5 h after HE addition, the red spectrum 13 h afterwards. The product formation could be observed, as well as a signal decrease of TRIM/Z-5, showing that a slow reaction occurs at 220 K. In all recorded spectra, no additional signals appeared over time (despite the formed product), indicating that no build up of the ternary complex proceeds.

11 Determination of the *E*-to-*Z*-isomerization rates

For the determination of the *E*-to-*Z*-isomerization rates $k_{E \rightarrow Z}$, the ΔG_{ges} has to be determined first. ΔG_{ges} arises from equation S13. The definition of ΔG_1 and ΔG_2 , which are used in this work, is depicted in figure S6.

$$\Delta G_1 + \Delta G_2 = \Delta G_{\text{ges}} \quad (\text{S13})$$

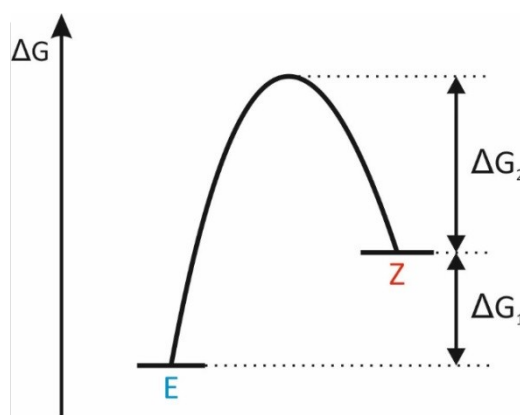


Figure S 15: The *E*-imine is thermodynamically more favored than the *Z*-imine. Additionally, the definition of the ΔG_1 and ΔG_2 used in this work is shown.

The only experimental way to determine the *Z*-to-*E*-isomerization rate is by increasing the amount of thermodynamically unfavored *Z*-imine by illumination with 365 nm (in-situ, for experimental set-up, see reference²²). Afterwards the back-isomerization to the more stable *E*-imine was observed with NMR. Finally, the decay-curves of the *Z*-imine can be fitted mathematically (with equation S14). The *Z*-to-*E*-isomerization rate is defined as $k_{Z \rightarrow E} = 1/t_1$. Then ΔG_2 can be calculated from equation S15. The obtained values are summarized in Table S7. The decay curves are shown in chapter 10.2.

$$y = A_1 * e^{\frac{-x}{t_1}} + y_0 \quad (\text{S14})$$

$$k_{Z \rightarrow E} = \frac{(k_B * T)}{h} * e^{-\frac{\Delta G_2}{RT}} \quad (\text{S15})$$

Table S 8: The experimentally observed *Z*-to-*E*-isomerization rates $k_{Z \rightarrow E}$, as well as the related ΔG_2 at different temperatures, are shown.

catalyst	imine	temperature [K]	$k_{Z \rightarrow E}$ [$*10^{-3}$ 1/s]	ΔG_2 [kJ]
TRIFP	5	230	2.52	67.28
TIPSY	5	230	1.19	68.71

TRIP	5	230	9.04	64.83
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For the determination of the *E*-to-*Z*-isomerization rate constants, the amount of *E*- and *Z*-imine in the binary complex was determined. Here it is very important that the spectra were recorded in the thermodynamic equilibrium. After some mathematical transformations of the Boltzmann distribution (equation S16), ΔG_1 can be observed from equation S17. Here, N_0 represents the integral of the *E*-imine, which is set to 1 in all cases. N_i is the integral of the *Z*-imine.

$$\frac{N_i}{N_0} = e^{\frac{-\Delta G_1}{k_B T}} \quad (\text{S16})$$

$$\Delta G_1 = -RT * \ln\left(\frac{N_i}{N_0}\right) \quad (\text{S17})$$

After the calculation of ΔG_{ges} (equation S13) the *E*-to-*Z*-isomerization rate $k_{E \rightarrow Z}$ can be determined with equation S18. The obtained values for ΔG_1 , ΔG_{ges} and $k_{E \rightarrow Z}$ are summarized in table S8 for different catalysts at 230 K.

$$k_{E \rightarrow Z} = \frac{(k_B * T)}{h} * e^{-\frac{\Delta G_{\text{ges}}}{RT}} \quad (\text{S18})$$

Table S 9: The experimentally observed amounts of *Z*-imine (N_i) and *E*-imine (N_0) as well as the calculated ΔG_2 , ΔG_{ges} and the *Z*-to-*E*-isomerization rates $k_{Z \rightarrow E}$ at 230 K in CD_2Cl_2 are shown.

catalyst	imine	T [K]	N_i	N_0	ΔG_1 [kJ]	ΔG_{ges} [kJ]	$k_{E \rightarrow Z}$ [$*10^{-3}$ 1/s]
TRIFP	5	230	0.1768	1	3.31	70.59	0.45
TIPSY	5	230	0.4786	1	1.41	70.11	0.57
TRIP	5	230	0.1500	1	3.63	68.46	1.36

11.1 Sample preparation

The catalyst (30 μmol) was directly weighed into a 5 mm NMR tube and dried for 20 min at 120°C under reduced pressure. Under argon atmosphere the Ketimine (30 μmol) was added and dissolved in dry CD_2Cl_2 (0.5 ml).

Even after careful sample preparation, partial hydrolysis of the imine could not be completely prevented. Therefore the imine/CPA-ratios are slightly different from 1:1.

11.2 Decay curves

The amount of *Z*-imine is increased by illumination with 365 nm with a glass fiber inside the NMR.^{18,22} For the imine **5** the photostationary state in CD₂Cl₂ at 190 K was reached after 3 h (constant *E/Z*-ratio of 1/1.7). Then the thermal *Z*-to-*E*-back-isomerization is observed inside the NMR-spectrometer at 230K. 230K were chosen because here the *Z*-imine is thermally back converted to the *E*-isomer in a reasonable amount of time. Over 250 K the back-isomerization is so fast that it could not be detected. All the measured decay curves as well as the associated fit-equations (see also equation S14) are shown in figure S7 to S9.

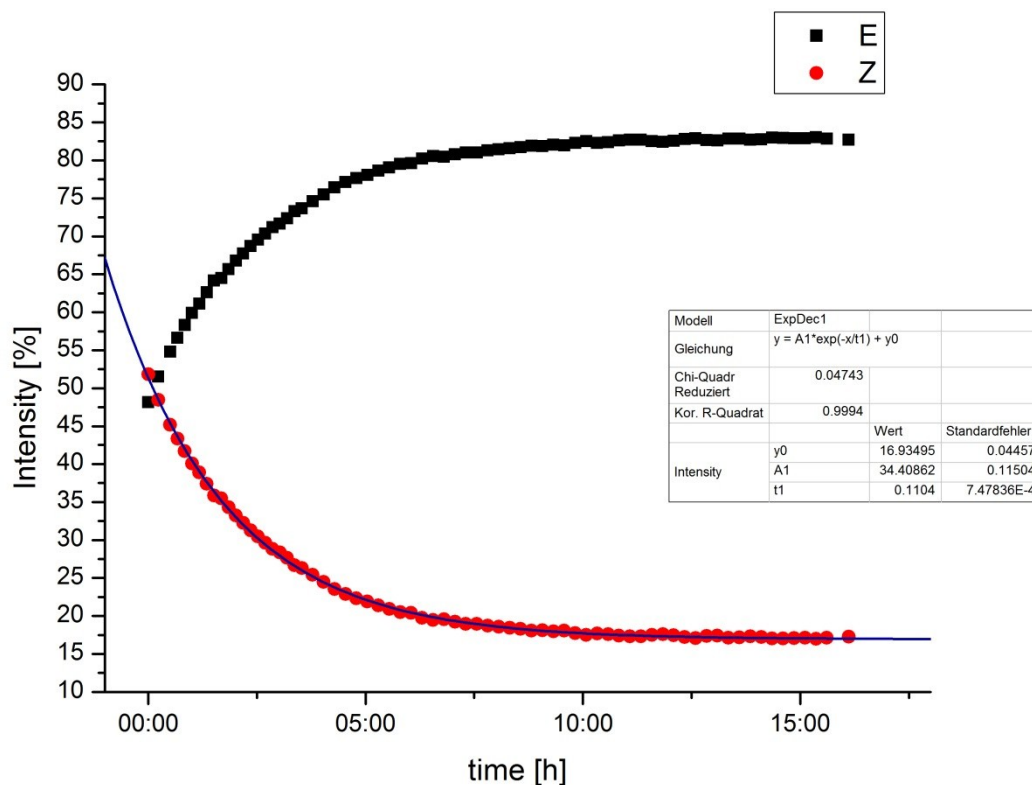


Figure S 16: The thermal back-isomerization of the *Z*-imine (red) in the binary TRIFP/**5**-complex at 230K in CD₂Cl₂ is shown. While the amount of *Z*-imine decreases, the amount of the thermodynamically more stable *E*-imine (black) is increased. The fit delivers the following values for the constants: $y_0 = 16.94 \pm 0.05$, $A_1 = 34.41 \pm 0.12$ and $t_1 = 0.1104 \pm 0.0008$.

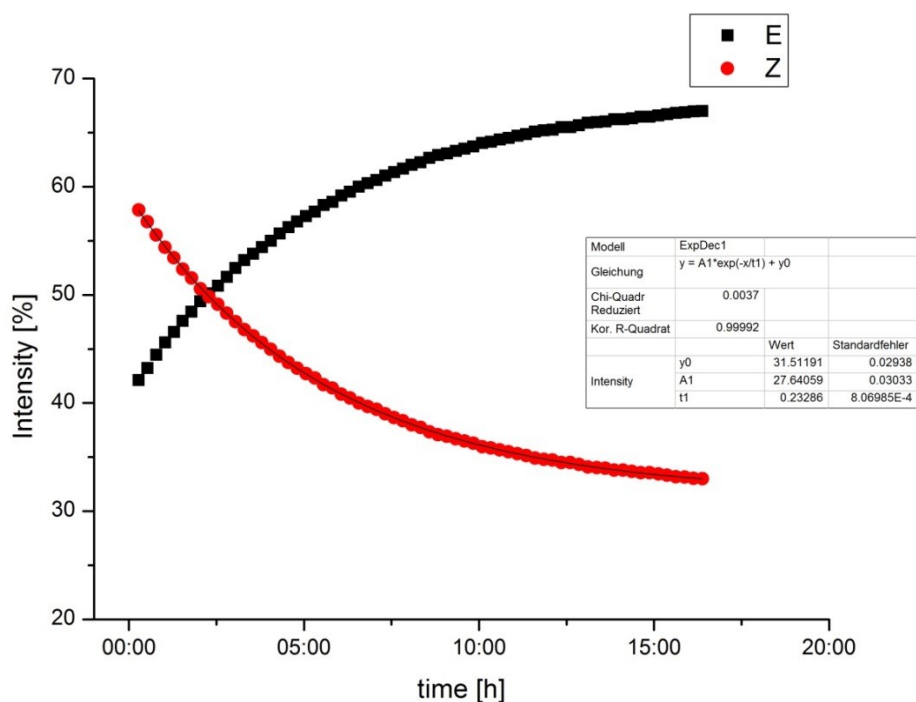


Figure S 17: The thermal back-isomerization of the Z-imine (red) in the binary TiPSY/5-complex at 230K in CD_2Cl_2 is shown. While the amount of Z-imine decreases, the amount of the thermodynamically more stable E-imine (black) is increased. The fit delivers the following values for the constants: $y_0 = 31.51 \pm 0.03$, $A_1 = 27.64 \pm 0.03$ and $t_1 = 0.2329 \pm 0.0008$.

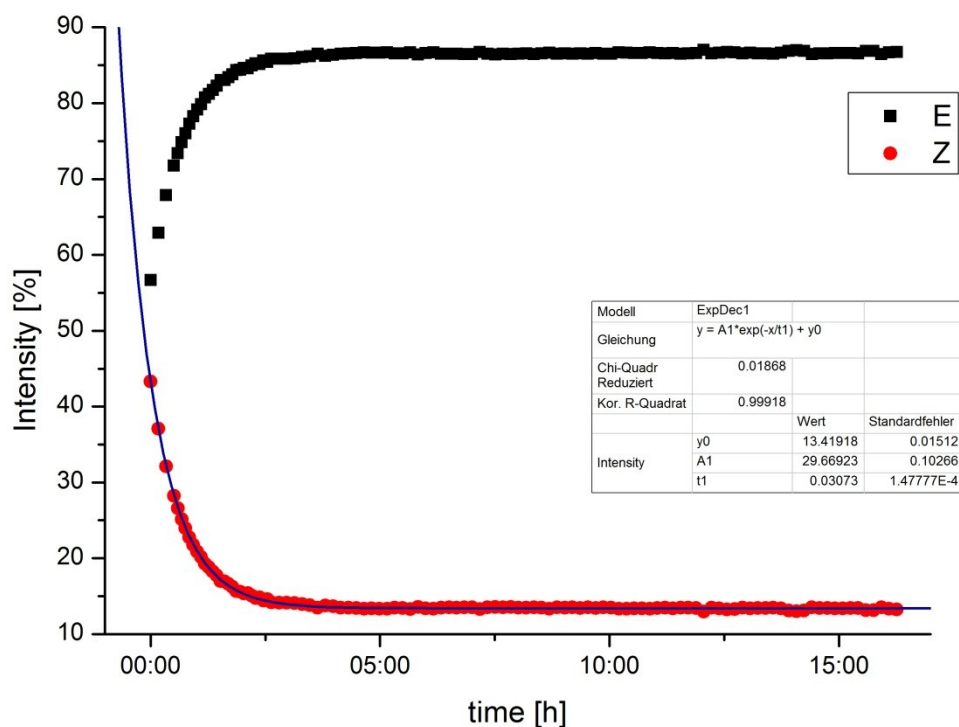


Figure S 18: The thermal back-isomerization of the Z-imine (red) in the binary TRIP/5-complex at 230K in CD_2Cl_2 is shown. While the amount of Z-imine decreases, the amount of the thermodynamically more stable E-imine (black) is increased. The fit delivers the following values for the constants: $y_0 = 13.41 \pm 0.02$, $A_1 = 29.67 \pm 0.10$ and $t_1 = 0.0307 \pm 0.0002$.

12 Investigations on the ternary complex of TRIP, imine **5** and Hantzsch ester

For the investigations of the ternary complex in this chapter, a TRIP/imine **5**/Hantzsch ester-ratio of 1:3:3 was used. This ratio was chosen to shift the equilibrium between the Hantzsch ester in its free form and the Hantzsch ester in the ternary complex to the side of the ternary complex.

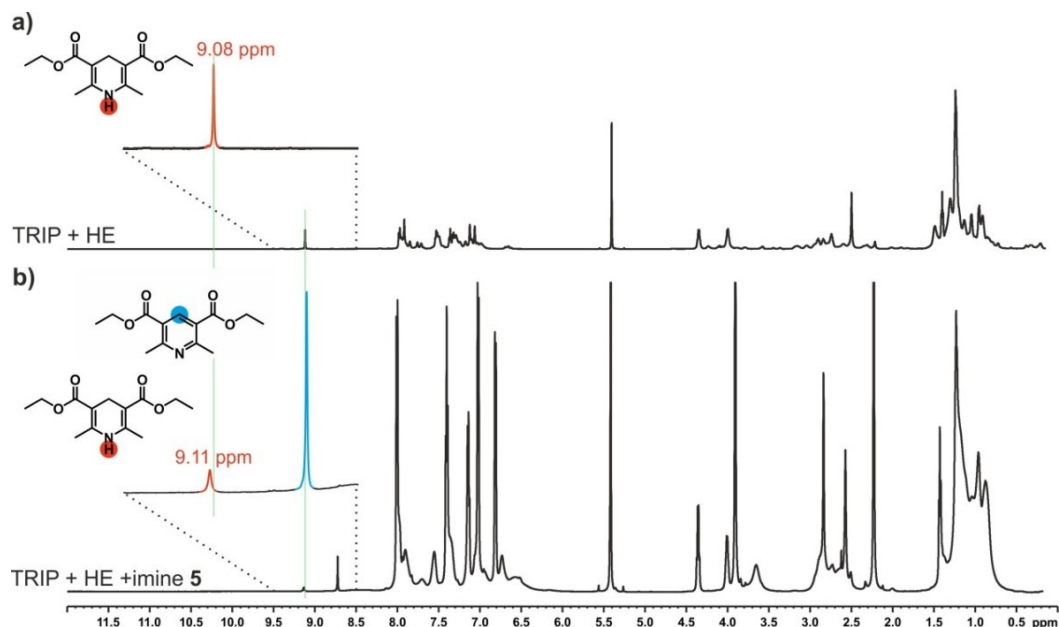


Figure S 19: The spectra of a) TRIP and Hantzsch ester (HE) and b) Hantzsch ester with TRIP and imine **5** in CD₂Cl₂ at 200K are shown. The very small shift ($\Delta\delta = 0.03$ ppm) of the NH-proton of the Hantzsch ester (red circle) in both spectra is a hint that only a small amount of ternary complex was formed. Both spectra are referenced to TMS.

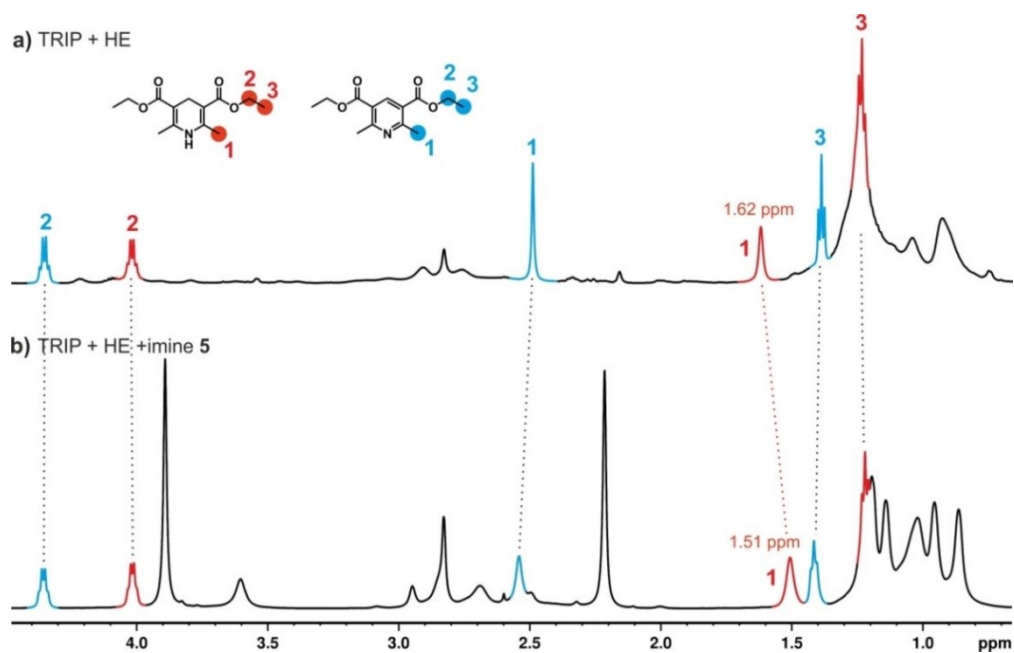


Figure S 20: The spectra of a) TRIP and Hantzsch ester (HE) and b) Hantzsch ester with TRIP and imine **5** in CD₂Cl₂ at 200K are shown. For the ortho-methyl group of the Hantzsch ester (red 1) a small highfield shift ($\Delta\delta = 0.51$ ppm) was observed. This may be due to the shielding by aromatic protons of the catalyst backbone. For the other aliphatic signals, almost no shift is observed. Both spectra are referenced to TMS.

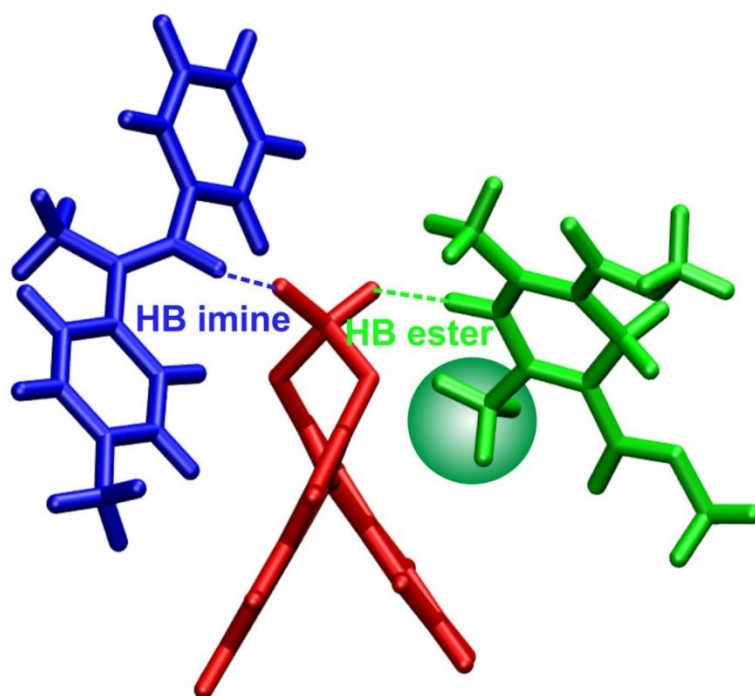
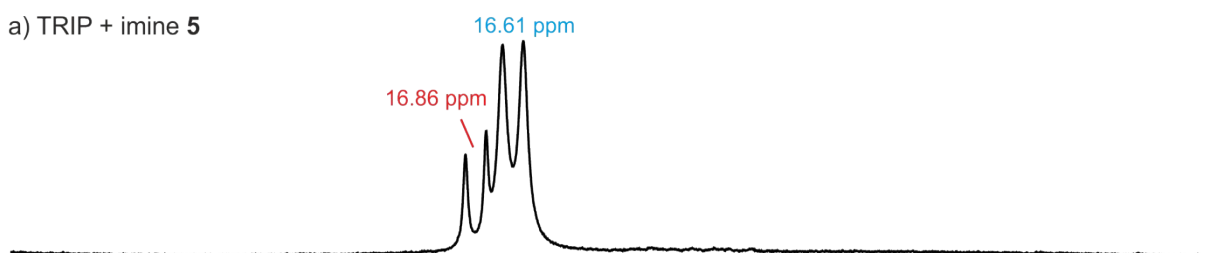


Figure S 21: Structural analysis of the computed ternary complex (imine **5**: blue, TRIP: red, Hantzsch ester: green) revealed spatial proximity of the *ortho*-methyl group (green circle) to the BINOL backbone of the TRIP which explains the high-field shift due to shielding by the aromatic ring. As an example, the *type I E*-imine **5** was chosen.

a) TRIP + imine **5**



b) TRIP + HE + imine **5**

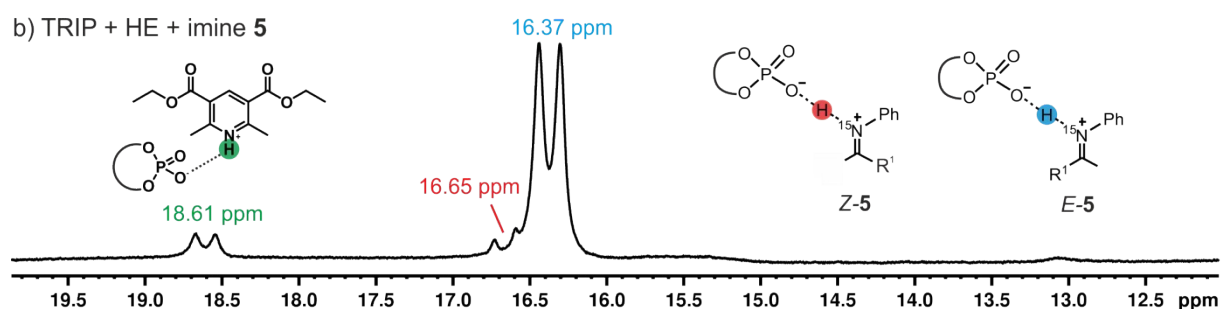


Figure S 22: a) The hydrogen bond region of the ^1H -spectra of imine **5** and TRIP (1:1) are (*E*-complex: 16.61 ppm and *Z*-complex: 16.86 ppm) b) After the addition of Hantzsch ester to imine **5** and TRIP both signals are slightly shifted (*E*-complex: 16.37 ppm and *Z*-complex: 16.65 ppm). Both spectra were recorded at 200 K in CD_2Cl_2 .

13 Investigations on the ternary complex of TRIM, imine **5** and Hantzsch ester

In the investigations of the ternary complex in this chapter a TRIM/imine **5**/Hantzsch ester-ratio of 1:1:1.4 was used.

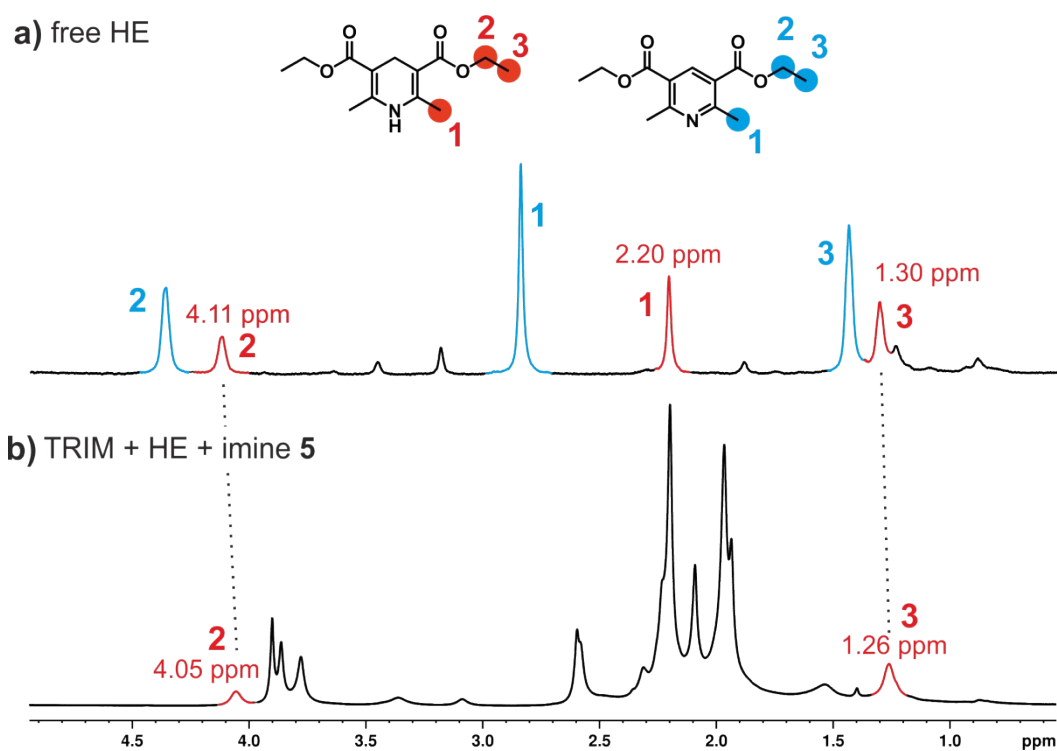


Figure S 23: The spectra of a) Hantzsch ester (HE) and b) Hantzsch ester with TRIP and imine **5** in CD_2Cl_2 at 180K are shown. For the signals 2 and 3 of the Hantzsch ester (red), small shift (for 2: $\Delta\delta = 0.06$ ppm and for 3: $\Delta\delta = 0.04$ ppm) could be observed. The assignment of proton 1 in spectrum b) is not unambiguous.

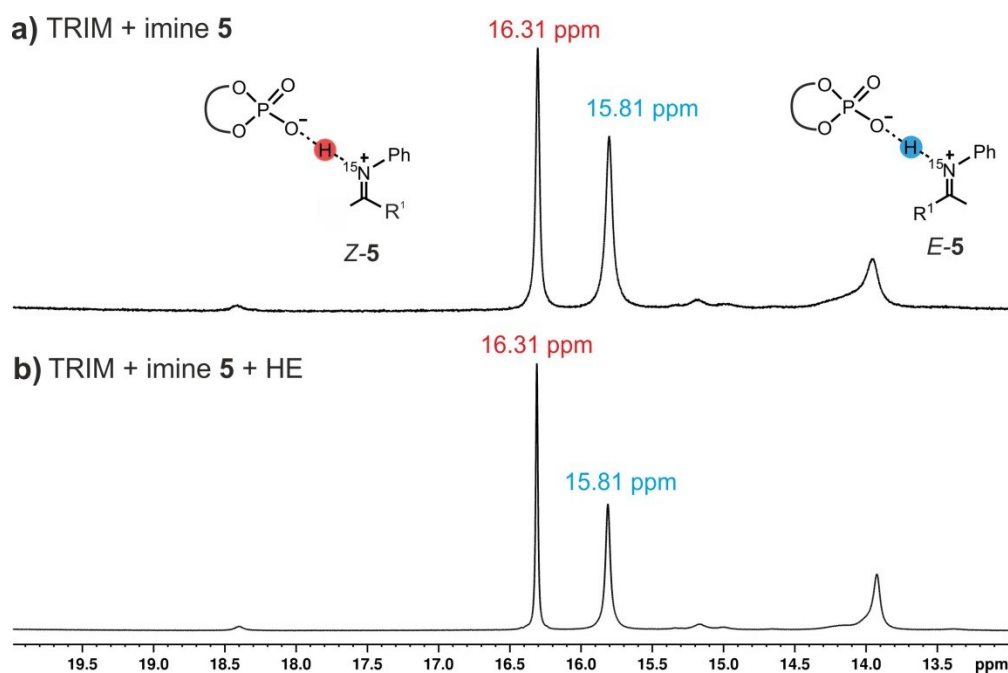


Figure S 24: a) In the spectra of imine **5** and TRIM the hydrogen-bonded protons of the E- and Z-complex (E-complex: 15.81 ppm and Z-complex: 16.31 ppm) are well separated. b) By adding Hantzsch ester to imine **5** and TRIM no shift of the signals is detectable (E-complex: 15.81 ppm and Z-complex: 16.31 ppm). Both spectra were recorded at 180 K in CD_2Cl_2 and referenced to TMS.

14 Barrier of the hydride transfer

According to the previous calculations, the barrier of hydride transfer equals 53 to 60 kJ/mol.¹⁸ Thus, under the assumption that the formation of the ternary complex is not rate limiting or thermodynamically unfavorable, the measured isomerization rate (barrier approx. 65 to 70 kJ/mol), is several order of magnitude slower than the hydride transfer step. The NMR spectra showed a fast exchange between the ternary complex and the binary complex. Hence, kinetically the formation of the ternary complex is not demanding; however, the minor shift of the Hantzsch ester acidic proton-signal suggests that the binding constant of Hantzsch ester is very low.

15 Solubility of Hantzsch ester in toluene

Hantzsch ester (14.50 mg, 0.057 mmol) was weighed into an NMR tube, and a solution of the standard (1,3,5-trimethoxybenzene, 2.88 mg, 0.017 mmol, 0.30 eq., 3.4 mM stock solution) in PhMe- d_8 (0.5 mL) was added. The sample was equilibrated at 308 K in the spectrometer for 15 min and ^1H NMR spectra (AQ: 10 s, pre-scan delay 2 s, 64 scans) of the dissolved Hantzsch ester were acquired on a 600 MHz instrument at 308 K (35 °C). The fast-relaxing methyl signals of the Hantzsch ester (δ 1.08 ppm) and the standard (δ 3.38 ppm) were integrated, and the concentration of the dissolved ester calculated.

Hantzsch ester from three different suppliers was used for this study for comparison. Some of the samples were stirred (600 rpm) in a Schlenk flask at 35 °C, treated with ultrasound (5 min) at 35 °C, or equilibrated for 1 h. In all cases, the concentration of the Hantzsch ester remained roughly constant at 2.0 – 3.1 mg.mL $^{-1}$ (8.0 – 12.4 mM).

16 Computational details

Binary complexes consist of TiPSY, TRIP, TRIFP and TRIM with imines **3**, **4**, **5** were optimized at TPSS-D3/def2-SVP level of theory in a continuum of CH₂Cl₂.^{23,24} 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.²⁵ Software used for the optimization was Gaussian09 D.01.²⁶ For single points, ORCA 4.1 was used.²⁷ For the basis set extrapolation procedure equation S19 – S21 were used with the basis set def2-SVP and def2-TZVP (X=2,3). $\alpha=10.39$, $\beta=2.40$.

$$E_{\text{SCF}}^X = E_{\text{SCF}}^{\infty} + Ae^{-\alpha\sqrt{X}} \quad (\text{S19})$$

$$E_{\text{corr,MP2}}^{\infty} = \frac{X^{\beta} E_{\text{corr,MP2}}^X - (X-1)^{\beta} E_{\text{corr,MP2}}^{X-1}}{X^{\beta} - (X-1)^{\beta}} \quad (\text{S20})$$

$$E_{\text{MP2}}^{\infty} = E_{\text{SCF}}^{\infty} + E_{\text{corr,MP2}}^{\infty} \quad (\text{S21})$$

For the calculation of external acidity, the structures are optimized at TPSS-D3/def2-SVP in the gas phase. A thermochemical correction was applied to the optimized geometry at the same level of theory. Solvent correction in DCM with a modified dielectric constant (16.20) to mimic low-temperature condition in the experiment was performed using SMD. Single points at SCS-MP2/CBS (using two points extrapolation from SVP and TZVP) were calculated on the optimized geometry. Software used for the geometry optimization was Gaussian09 D01, and for the single points, ORCA 4.1 was used.

17 Optimized geometry of most stable conformations

TRIP/3 Type I E

```
1\1\GINC-LOGINF\Opt\RTPSSTPSS\def2SVP\W06\C65H72N1O4P1\JHIOE\20-Dec-20
14\0\#p opt tpsstps\def2svp\w06 densityfit empiricaldispersion=gd3 s
crf=(smd,solvent=ch2cl2,read)\title\0,1\p,-0.1011446316,-0.381696061
9,-1.3053979587\O,-1.3822205925,0.6833982565,-1.4840537197\O,0.8261569
238,0.4942645244,-0.1829509614\O,0.5563266402,-0.4716094397,-2.6505793
637\O,-0.5213671571,-1.5974615169,-0.4855823064\C,-1.2551259372,2.3460
146336,0.2328614085\C,-1.9467616045,1.3020957171,-0.3890764233\C,-3.26
17405104,0.8936664028,-0.0005778465\C,-3.8595223409,1.5585199933,1.061
9581279\H,-4.8753214905,1.2848511886,1.3655159574\C,-3.1739990527,2.56
69865261,1.797837331\C,-1.8420301097,2.954865256,1.4019800193\C,-1.142
3848445,3.8919479964,2.2214028534\H,-0.1141332608,4.1615451233,1.96492
31962\C,-1.7376376598,4.4468599707,3.344949566\H,-1.175092692,5.156129
2462,3.9620101474\C,-3.0664190836,4.0972562364,3.7065411205\H,-3.52790
65596,4.5474932508,4.5921384707\C,-3.7653967878,3.1712557218,2.9482729
763\H,-4.7816409884,2.8729632748,3.2301642429\C,0.0782502652,2.7703599
429,-0.2831085757\C,1.100635401,1.8250850793,-0.416500735\C,2.45779191
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7\H,3.7753307261,3.8153434064,-1.1525996677\C,1.7187251932,4.504781433
6,-0.9769922452\C,0.3648476838,4.1381299387,-0.63931265\C,-0.645058534
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\C,-0.3327534006,6.4486454497,-1.0650711833\H,-1.1268808491,7.20144178
73,-1.1203611332\C,1.0063261264,6.8143282506,-1.3672265366\H,1.2409405
901,7.8483668756,-1.6425671338\C,2.0089175009,5.8581535128,-1.32557488
18\H,3.043466893,6.1238995476,-1.5712622337\C,-1.584151431,-0.64247980
26,4.5774403118\C,-1.1209128973,-1.8865528692,5.0549787737\H,-1.503949
8434,-2.2767570046,6.0043300726\C,-0.1792602886,-2.6331463375,4.339347
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01039,3.0893781958\C,-0.154265571,-0.9187481673,2.6116485325\H,0.22824
48496,-0.5116869762,1.6730956645\C,-1.0666851908,-0.169357515,3.351355
864\H,-1.3895311471,0.8027625269,2.9662789967\C,1.252029221,-2.9835153
298,2.3179290403\C,2.2362075586,-3.8582277046,3.0352006532\H,3.1457525
741,-4.0098473292,2.4327018419\H,1.791456013,-4.8500982998,3.235886793
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TRIP/3 Type II E

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TRIP/3 Type II Z

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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/4 Type I E

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TRIP/4 Type II E

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TRIP/4 Type I Z

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TRIP/4 Type II Z

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TiPSY/3 Type I E

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TIPSY/3 Type II E

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TIPSY/3 Type I Z

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TIPSY/3 Type II Z

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TIPSY/5 Type I E

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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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23.8576271,34.5447013,-7.9584256,-4.4817681\PG=C01 [X(C71H56N1O5P1Si2)
]\@

TIPSY/4 Type I E

1\1\GINC-LOGIN\FOpt\RTPSSTPSS\def2SVP/W06\C71H53F3N1O4P1Si2\JHIOE\15-N
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792498\O,-0.2237964717,-1.7412289197,-0.6475216795\C,-0.7537158599,2.3
046376891,-0.0821949946\C,-1.5165301831,1.3111157578,-0.7012917839\C,-
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2.8628573173,1.2869276841\C,-1.3555344215,3.051349792,0.9983764847\C,-
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486912306\C,-1.2283012039,4.6458022994,2.8549312827\H,-0.6342583681,5.
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TiPSY/4 Type II E

1\1\GINC-WORKER1\FOpt\RTSPSS\def2SVP\W06\C71H53F3N1O4P1Si2\JHIOE\01-
Dec-2016\0\#p opt scrf=(smd,solvent=ch2cl2,read) tpsstps/def2svp/w0
6 densityfit empiricaldispersion=gd3\title\0,1P,0.1441088148,0.4612
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79,3.4619182769,4.6131828152\H,-0.2402616931,3.3046104527,5.084939468\N,-0.1109924455,1.3246636996,2.8504695302\H,0.1442594396,1.2125811076,1.7999844088\C,0.3837209997,0.2383147142,3.6246346482\C,0.4833022185,-0.9936299995,2.9421853097\H,0.1572633417,-1.0570876796,1.9001787144\C,0.9808948948,-2.1165525082,3.6092852641\H,1.0455804046,-3.0716153105,3.0793817216\C,1.3995571922,-2.0168591815,4.9458184175\C,1.3290051615,-0.7824125308,5.6100017618\H,1.6795279602,-0.692314476,6.6433457878\C,0.8283034839,0.35237457,4.9577560181\H,0.826787382,1.3119729591,5.4757175282\H,1.7940073229,-2.8971988843,5.4639430705\C,-1.8206440553,5.977171648,-1.2409876279\Si,4.1421168418,0.5066065877,-0.6548601617\Si,-3.9199474187,-1.1382798031,-0.4126025396\C,5.6637126206,0.0841488703,-1.7152237969\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,6.0056189412,1.5712015589,1.3208041611\C,4.1031291425,1.6384143269,3.3807392038\H,2.7248544652,0.8187748291,1.9253350966\C,6.364962073,2.046109864,2.5934174725\H,6.7626352912,1.5468321331,0.5275901683\C,5.4138580485,2.0815098501,3.6253379586\H,3.3557657711,1.6584486419,4.182102032\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\RMSE=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/4 Type I Z

1\1\GINC-LOGIN\FOpt\RTPSSSTPSS\def2SVP\W06\C71H53F3N1O4P1Si2\JHIOE\19-Nov-2015\0\#p tpsstps\def2svp\w06 densityfit empiricaldispersion=gd3 opt scrf=(smd,solvent=ch2cl2,read)\title\0,1\p,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,-2.9856981777,3.1766

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53F3N1O4P1Si2)]\@

TiPSY/4 Type II Z

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TRIFP/3 Type I E

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TRIFP/3 Type II E

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TRIFP/3 Type II Z

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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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O5P1)]\@

TRIFP/5 Type II Z

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TRIFP/4 Type I E

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TRIFP/4 Type II E

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TRIFP/4 Type I Z

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TRIFP/4 Type II Z

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TRIM/3 Type I E

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TRIM/3Type II E

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TRIM/3 Type I Z

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TRIM/3Type II Z

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TRIM/5 Type I E

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TRIM/5 Type II E

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78,-3.7770531,-11.5491766,-4.2608599,-16.0409702\PG=C01 [X(C53H48N1O5P
1)]\@

TRIM/5 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
,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\
C,-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
6336341,6.7155058426,-0.2146028399\C,4.925782249,-2.5530092491,3.83338

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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
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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,6.0040942086,-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
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7e-06\Dipole=4.0253688,-2.7545032,4.7228696\Quadrupole=5.6749485,3.162
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1)]\@

TRIM/5Type II Z

1\1\GINC-LOGIN\Opt\RTPSSTPSS\def2SVP\C53H48N1O4P1\JHIOE\26-Jul-2018\0
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176097658,-0.475648838\O,-0.5186893,0.4696256823,-2.9945337106\O,-1.00
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56435565\C,-2.3830695381,0.9577767616,0.3025340357\C,-3.5105827685,0.2
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,-0.3577735763,-0.1498570115\C,-4.3713129955,-0.5521565352,-0.17706180
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,-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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-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
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,-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\
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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
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\Dipole=4.4526636,-3.1427545,3.5680717\Quadrupole=12.8721156,4.3863326
,-17.2584483,-21.5761061,-6.4216927,2.5011674\PG=C01 [X(C53H48N1O4P1)]
\@

TRIM/4 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
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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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1479310054,2.6398172466,1.4147093142\H,-2.4015820439,3.3783703566,1.1
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30717,-2.0743162615,0.6296475869\C,3.8372874363,-1.7822907395,-0.74294
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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
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6434318582\C,-3.6149273442,-4.208161617,-2.6702488819\C,-3.1235519966,
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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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708,1.9167647676,-0.2678432508\H,6.75068237,0.2385995626,-0.0579303695
\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,
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ole=21.4170786,-10.0017465,-11.4153321,-13.0753119,21.9535418,-7.99031
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TRIM/4 Type II E

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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,

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,1.5943780889,4.9570799651,-0.7978734575\C,-0.5508264816,4.596012574,-
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,0.3142902082,-1.8511404682,2.7824219079\C,-0.6379627048,-0.8215491559
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,2.5887551912,2.4601595837,-0.2957070629\C,3.450865982,2.3599837055,-
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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
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TRIM/4 Type I Z

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,0.614127009,-0.4737541777\O,-0.6032920756,0.3557444103,-2.950936586\O
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,1.1514785431\C,-2.3907532762,0.9133267788,0.3787113357\C,-3.446006128
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1)]\@

TRIM/4 Type II Z

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