Titanium-catalyzed esterification reactions: beyond Lewis acidity

Lukas A. Wolzak, Jarl Ivar van der Vlugt, Keimpe J. van den Berg, Joost N. H. Reek,* Moniek Tromp,* and Ties J. Korstanje*
Supplementary Materials for

Titanium-catalyzed esterification reactions: beyond Lewis acidity

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Materials and Methods

General

Dichloromethane and acetonitrile were distilled from CaH₂, n-pentane and Et₂O from sodium/benzophenone and toluene from sodium under argon atmosphere. Ethanol was degassed and dried over 3Å molecular sieves. All other chemicals were obtained from Merck or Fluorochem and were used without further purification. All air-sensitive materials were manipulated using standard Schlenk techniques or by the use of an argon-filled glovebox (MBraun Unilab). The NMR solvents CD₂Cl₂, toluene-δ₈ and C₆D₆ were dried over molecular sieves and degassed via three cycles of freeze-pump-thaw. ¹H spectra were recorded on a 300 or 400 MHz Bruker AVANCE spectrometer and ¹³C NMR on 125 or 100 Mhz respectively. Spectra were referenced against residual solvent signal. FD-MS spectra were collected on an AccuTOF GC v 4g, JMS-T100GCV Mass spectrometer (JEOL, Japan) equipped with a Carbotec emitter. A typical current rate of 51.2 mA/min over 1.2 min and a flashing current 40 mA on every spectra of 30 ms was used. High resolution ESI-MS spectra were recorded on a JEOL AccuTOF LC-Plus JMS-T100LP spectrometer in CH₃CN. IR spectra were recorded on a Bruker Alpha FTIR machine. GC analysis for heptylbenzoate and benzoic acid was performed on a Thermo Scientific Trace GC Ultra equipped with a Restek stabilwax-DA column (30 m x 0.25 mm x 0.25 μm). Temperature program: initial temperature 50 °C, heat to 200 °C with 20 °C min⁻¹, hold for 10 min, heat to 250°C with 50 °C min⁻¹, hold for 3 minutes. Inlet temperature 250 °C, split ratio of 30, 1.0 mL min⁻¹ helium flow, FID temperature 250 °C. Esterification reactions were performed in a Radley Discoveries 12 plus reaction station allowing a maximum of 12 simultaneous reactions under a nitrogen atmosphere.
Single crystal X-ray diffraction

X-ray Crystal Structure Determination of complex 11: X-ray intensities were measured on a Bruker D8 Quest Eco diffractometer equipped with a Triumph monochromator (λ = 0.71073 Å) and a CMOS Photon 100 detector at a temperature of 150(2) K. Intensity data were integrated with the Bruker APEX3 software.\(^1\) Absorption correction and scaling was performed with SADABS.\(^2\) The structures were solved using intrinsic phasing with the program SHELXT.\(^3\) Least-squares refinement was performed with SHELXL-2014\(^4\) against F2 of all reflections. Non-hydrogen atoms were refined with anisotropic displacement parameters. The H atoms were placed at calculated positions using the instructions AFIX 13, AFIX 43 or AFIX 137 with isotropic displacement parameters having values 1.2 or 1.5 times Ueq of the attached C atoms. CCDC 1941519 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Computational details

Geometry optimizations were carried out with the Amsterdam Density Functional (ADF) program package using version 2017.201.\(^5\),\(^6\) We used the BP86 functional in combination with the TZ2P basis set and a large frozen core.\(^7\),\(^8\),\(^9\) Grimme’s dispersion corrections (version 3, disp3) were used to include Van der Waals interactions.\(^10\) All minima (no imaginary frequencies) and transition states (one imaginary frequency) were characterized by calculating the Hessian matrix. ZPE and gas-phase thermal corrections (enthalpy, 298 K) from these analyses were calculated.
Experiments

**Catalytic esterification of benzoic acid with heptanol**

In a carousel reaction station under a nitrogen atmosphere benzoic acid (610.6 mg, 5 mmol) was dissolved in heptanol (7.14 mL, 50 mmol). Two different runs were performed, for the catalyzed reactions 1 mol% catalyst was used. To half of the reaction mixtures 1 g of activated powdered 4 Å molecular sieves were added and for all samples pentadecane (0.41 mL, 1.5 mmol) was used as internal standard. Samples for GC analysis were taken after 3 h, 6 h, 10 h and 24 h (averaged over 2 runs).

![Figure S1. Catalytic results of the esterification of benzoic acid with heptanol (1:10 ratio) using no catalyst, titanium(IV) isopropoxide or complex 10 as catalyst, either in the presence or absence of molecular sieves.](image-url)
Determination of order of reaction

In a carousel reaction station under a nitrogen atmosphere benzoic acid (610.6 mg, 5 mmol) was dissolved in heptanol (7.14 mL, 50 mmol). Two different runs were performed with complex 10 added as a powder (0.25, 0.5, 1 and 1.5 mol%) and pentadecane (0.41 mL, 1.5 mmol) as internal standard. Samples for GC analysis were taken after 1 h and 2 h. The rate (mol/L*s) was determined via a tangent line of the heptyl benzoate concentration between 1 h and 2 h.

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Table S1. Reaction rate between 1 h and 2 h at various catalyst loadings
**Determining activation energy**

In a carousel reaction station under a nitrogen atmosphere benzoic acid (610.6 mg, 5 mmol) was dissolved in heptanol (7.14 mL, 50 mmol). Complex 10 was added as a powder (21.97 mg, 1 mol%) and pentadecane (0.41 mL, 1.5 mmol) as internal standard. Four different runs were performed in duplo at 150 °C, 160 °C, 170 °C and 180 °C and samples for GC analysis were taken after 1 h and 2 h. The rate (mol/L*s) was determined via a tangent line of the heptyl benzoate concentration between 1 h and 2 h. The activation energy is given by $10108 \times 8.3145 = 84.04$ KJ/mol or 20.09 Kcal/mol

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**Figure S2.** Order in catalyst
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**Table S2.** Reaction rate between 1h and 2h at various temperatures

**Figure S3.** Arrhenius plot: the activation energy is given by $10141 \times 8.3145 = 84.32 \text{ KJ/mol}$ or $20.15 \text{ Kcal/mol}$
Figure S4: $^1$H NMR of 7, CD$_2$Cl$_2$
Figure S5: $^{13}$C NMR of 7, CD$_2$Cl$_2$
Figure S6: $^1$H $^{13}$C HSQC NMR of 7, CD$_2$Cl$_2$
Figure S7: $^1$H NMR of 11, CD$_2$Cl$_2$
Figure S8: $^1$H NMR of 11 upon addition of D$_2$O, CD$_2$Cl$_2$
Figure S9: $^{13}$C NMR of 11, CD$_2$Cl$_2$
Figure S10: $^1$H $^{13}$C HSQC NMR of 11, CD$_2$Cl$_2$
Figure S11: VT $^1$H NMR (193 to 293 K) of 11, tol-$d_8$. Methylene protons indicated with a red dot.
Figure S12: $^1$H NMR of 12, CD$_6$. Acetic acid signals indicated with a red dot.
Figure S13: $^1$H NMR of 13, C$_6$D$_6$
Figure S14: $^{13}\text{C}$ NMR of 13, C$_6$D$_6$
Figure S15: $^1$H $^{13}$C HSQC NMR of 13, C$_6$D$_6$
Figure S16: $^1$H COSY NMR of 13, C$_6$D$_6$
Figure S17: $^1$H NMR of 6 after reaction with acetic acid and ethanol, CD$_2$Cl$_2$. 
Figure S18: FD-MS of 7
Figure S19: FD-MS of 11
Figure S21: FD-MS of 13
Figure S22: FD-MS of esterification reaction catalyzed by complex 6 (after 30 min reaction time)
Figure S23: ATR IR spectrum of 11
Figure S24: Alternative, higher lying, reaction pathways for the esterification of acetic acid and ethanol catalyzed by complex 10
Cartesian coordinates (XYZ) for all calculated DFT structures

Intermediate A

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Intermediate B

$E$ (Hartree) $\quad -14.046788720757005$

$G_{298}$ (Hartree) $\quad -13.662004760895424$

$\Delta E$ (kcal mol$^{-1}$) $\quad 7.34$

$\Delta G_{298}$ (kcal mol$^{-1}$) $\quad 7.58$

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ΔG_{298} (kcal mol⁻¹)  10.04

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O  -0.95540371  -0.21239236  -2.96887104
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C  -1.20186588  -1.35234932  1.69823293
C  -1.68557654  -1.97072323  2.85822245
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C  -1.76746638  -3.21894978  4.07247041
H  -2.1523196  -1.79819781  4.95640235
C  -1.34415725  0.00299833  4.1451546
H  -1.39859217  0.58211130  5.08861541
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C  -1.23990727  -2.13178086  0.40641713
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G_{298} (Hartree)    -15.303149597654818
ΔE (kcal mol⁻¹)      1.92
ΔG_{298} (kcal mol⁻¹) 16.84

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O   0.67843115  0.56036425  -3.00742483
O   -2.06287020 0.48110323   -2.49482350
N  -0.45291407 -1.91697765  -2.15499704
C   1.15718342 -1.48121093   0.37799914
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C   0.80140857 -3.82709545   0.83184038
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C   1.74020737 -3.79093446   1.86198676
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G\text{298} (Hartree)  -15.295022200576598
\Delta E (\text{kcal mol}^{-1})  5.18
\Delta G\text{298} (\text{kcal mol}^{-1})  21.94
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G_{298} \text{ (Hartree)} & \quad -15.2989163206175594 \\
\Delta E \text{ (kcal mol}^{-1}\text{)} & \quad 3.13 \\
\Delta G_{298} \text{ (kcal mol}^{-1}\text{)} & \quad 19.49
\end{align*} \]

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$G_{298}$ (Hartree)  -15.293006214247281
$\Delta E$ (kcal mol$^{-1}$)  7.53
$\Delta G_{298}$ (kcal mol$^{-1}$)  23.20

68

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\end{array}$
Intermediate F

\[ E \text{ (Hartree)} = -15.761629925911334 \]
\[ G_{298} \text{ (Hartree)} = -15.301816401725974 \]
\[ \Delta E \text{ (kcal mol}^{-1} \text{)} = 2.87 \]
\[ \Delta G_{298} \text{ (kcal mol}^{-1} \text{)} = 17.67 \]
Intermediate G

\[ E \text{ (Hartree)} = -15.223672912752560 \]
\[ G_{298} \text{ (Hartree)} = -14.786843188214558 \]
\[ \Delta E \text{ (kcal mol}\(^{-1}\)) = 14.06 \]
\[ \Delta G_{298} \text{ (kcal mol}\(^{-1}\)) = 16.31 \]

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G_{298} (Hartree)  -1.673931413550113

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C  -1.45143729  0.71484444  0.00000000
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Ethanol

E (Hartree)  -1.707720569515242
G_{298} (Hartree)  -1.655900468654750

O  3.71777994  0.00578685  0.07852645
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H  1.67173486  -1.24259967  -1.03762573
H  1.48034928  -1.24258788  0.73123591
Ethyl acetate

E (Hartree)  -2.898787279654650
G_{298} (Hartree) -2.815573720215513

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Water

E (Hartree)  -0.520115002440625
G_{298} (Hartree) -0.517139017008766

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Intermediate A\textsubscript{NO2}

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O   -0.40627672  0.82542085  0.11580295
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C   -3.36852300 -1.63981192  -0.90003980
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C   2.70809638  -1.14043912  2.88463794
O   4.60337977  -1.32816506  4.21353538
C   3.14793821  0.08414290  2.37640720
H   4.09765662  0.49090869  2.71586002
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\end{verbatim}

### Transition state AB-NO2

![Transition state AB-NO2](image)

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\Delta G_{298} \text{ (kcal mol}^{-1}\text{)} & = 16.39
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$$G_{298} \text{ (Hartree)} = -17.008127046025091$$

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$$\Delta G_{298} \text{ (kcal mol}^{-1}\text{)} = 21.22$$

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$\Delta G_{298}$ (kcal mol$^{-1}$) 19.13

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Intermediate $F_{\text{NO}_2}$

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$G_{298}$ (Hartree) \hspace{1cm} -17.016374997695802
$\Delta E$ (kcal mol$^{-1}$) \hspace{1cm} 2.74
$\Delta G_{298}$ (kcal mol$^{-1}$) \hspace{1cm} 16.04

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**Notes:**
- Each cell represents a specific coordinate value in a 3D space.
- The columns likely correspond to different dimensions (X1, X2, X3, X4).
- The values are presumably floating-point numbers representing coordinates.
- The table format helps in visualizing the data's layout and structure.
Intermediate $G^{\text{NO2}}$

$E$ (Hartree) -16.936261283326459

$G_{298}$ (Hartree) -16.501949473182655

$\Delta E$ (kcal mol$^{-1}$) 12.21

$\Delta G_{298}$ (kcal mol$^{-1}$) 14.34

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\[ \Delta E (\text{kcal mol}^{-1}) = 0.00 \]
\[ \Delta G_{298} (\text{kcal mol}^{-1}) = 0.00 \]

71

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| C   | 0.18460858   | -2.93202525 | 0.55068713  |
| C   | 0.38945011   | -4.19789874 | 1.09887108  |
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Transition state $\text{AB-OMe}$

$E$ (Hartree) $-16.529400299428946$

$G_{298}$ (Hartree) $-16.055769416101541$

$\Delta E$ (kcal mol$^{-1}$) $12.72$

$\Delta G_{298}$ (kcal mol$^{-1}$) $13.03$

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Intermediate B-OMe

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G_{298} \text{(Hartree)} &\quad -16.067395364637232 \\
\Delta E \text{(kcal mol}^{-1} \text{)} &\quad 7.38 \\
\Delta G_{298} \text{(kcal mol}^{-1} \text{)} &\quad 6.66
\end{align*}
\]

\[
\begin{align*}
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\[ \Delta E \text{ (kcal mol}^{-1}\text{)} = -11.99 \]
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\[ G_{298} \text{ (Hartree)} = -17.708028200718587 \]
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$$\Delta G_{298} \text{ (kcal mol}^{-1}\text{)} = 16.06$$

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ΔG_{298} (kcal mol$^{-1}$) 22.58
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$$G_{298} \ (\text{Hartree}) = -17.704205725667261$$
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$$\Delta G_{298} \ (\text{kcal mol}^{-1}) = 18.63$$

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Transition state EF-OMe

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E \text{ (Hartree)} &= -18.244313151128704 \\
G_{298} \text{ (Hartree)} &= -17.697871697968043 \\
\Delta E \text{ (kcal mol}\(^{-1}\)) &= 8.21 \\
\Delta G_{298} \text{ (kcal mol}\(^{-1}\)) &= 22.61
\end{align*}
\]

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\]
### Intermediate FOMe

![Intermediate FOMe](image)

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- **E (Hartree)**: -18.252117090257485
- **G298 (Hartree)**: -17.706768191013893
- **ΔE (kcal mol\(^{-1}\))**: 3.31
- **ΔG298 (kcal mol\(^{-1}\))**: 17.02


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Intermediate G_{OMe}

![Image of a molecular structure](image)

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Alternative reaction pathways

Intermediate I

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ΔG<sub>298</sub> (kcal mol<sup>-1</sup>)  3.35

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\Delta E (\text{kcal mol}^{-1}) & = 7.60 \\
\Delta G_{298} (\text{kcal mol}^{-1}) & = 23.48 \\
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G_{298} \text{ (Hartree)} \quad -15.292679250387289 \\
\Delta E \text{ (kcal mol}^{-1}\text{)} \quad 7.07 \\
\Delta G_{298} \text{ (kcal mol}^{-1}\text{)} \quad 23.41
\]

68

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Transition state_{JK1}

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G_{298} (Hartree) -15.272411884144013
ΔE (kcal mol^{-1}) 20.58
ΔG_{298} (kcal mol^{-1}) 36.13

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### Intermediate $K_i$

- $E$ (Hartree): $-15.739065436500381$
- $G_{298}$ (Hartree): $-15.280109780344695$
- $\Delta E$ (kcal mol$^{-1}$): $17.03$
- $\Delta G_{298}$ (kcal mol$^{-1}$): $31.30$

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Transition state \( \text{JK2} \)

\[
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E (\text{Hartree}) & \quad -15.745654864679437 \\
G_{298} (\text{Hartree}) & \quad -15.281935766142839 \\
\Delta E (\text{kcal mol}^{-1}) & \quad 12.89 \\
\Delta G_{298} (\text{kcal mol}^{-1}) & \quad 30.15
\end{align*}
\]

68

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Intermediate $K_2$

$E$ (Hartree) \quad -15.760465006691440
$G_{298}$ (Hartree) \quad -15.293993266563952
$\Delta E$ (kcal mol$^{-1}$) \quad 3.60
$\Delta G_{298}$ (kcal mol$^{-1}$) \quad 21.27

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\begin{tabular}{ccc}
Ti & 0.19166544 & 0.45039173 & -0.01411809 \\
O & -1.50969937 & 0.27307089 & 0.94922049 \\
O & 1.33217747 & -0.07340610 & 1.35898464 \\
O & 1.39023427 & 0.16315266 & -1.45947300 \\
N & -0.20118679 & -1.90064800 & -0.23692658 \\
H & -1.97721318 & 1.98455637 & 0.94931903 \\
H & 3.65350978 & -0.08448798 & 2.50575184 \\
C & -0.85247132 & 4.21301410 & 2.94216474 \\
O & -0.19451408 & 3.25252099 & 2.09502778 \\
H & -0.40955181 & 5.21234466 & 2.78970724 \\
H & -1.92216722 & 4.26645646 & 2.68451985 \\
C & -0.65984173 & 3.75429039 & 4.37582255 \\
H & 0.40836835 & 3.6789105 & 4.61501005 \\
H & -1.11638356 & 2.76819177 & 4.52721459 \\
C & -1.56334984 & -2.15869449 & -0.76820902 \\
H & -1.69041805 & -3.25021207 & -0.90017551 \\
H & -1.59447105 & -1.70559727 & -1.76737025 \\
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C & 1.30332927 & -2.43296856 & 1.71257672 \\
C & 1.96846012 & -3.56365053 & 2.19518250 \\
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C & 3.22323914 & -3.46406141 & 2.79762030 \\
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H & -0.79708363 & -2.01671557 & 1.76681767 \\
C & 1.19158896 & -0.52203162 & -2.59371474 \\
\end{tabular}
Literature


