Supporting Information

for

Discovery and Mechanistic Study of Al\textsuperscript{III}-Catalyzed Transamidation of Tertiary Amides

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Contents:

Full citation for Gaussian 03 \hspace{1cm} S1

\textsuperscript{1}H NMR spectra of substrates, Al\textsubscript{2}(NMe\textsubscript{2})\textsubscript{6} and their combinations at 90 °C in toluene-\textit{d}\textsubscript{8} \hspace{1cm} S2

\textsuperscript{1}H NMR spectra of substrates, Al\textsubscript{2}(NMe\textsubscript{2})\textsubscript{6} and their combinations at 28 °C in toluene-\textit{d}\textsubscript{8} \hspace{1cm} S3

Full listings of calculated Cartesian geometries, energies and unique imaginary frequencies (for transition state structures) \hspace{1cm} S4-S18

Full citation for ref 16:

Figure S1. $^1$H NMR spectra of various combinations of amine and carboxamide substrates and the Al$_2$(NMe$_2$)$_6$ catalyst at 90 °C in toluene-$d_8$. These spectra provide additional benchmarks for the interpretation of $^1$H NMR spectra acquired during Al$^{III}$-catalyzed transamidation of tertiary amides (cf. Figure 6 in the manuscript). (IS = internal standard = trimethoxybenzene; S = solvent = toluene-$d_8$).
Figure S2. $^1$H NMR spectra of various combinations of amine and carboxamide substrates and the Al$_2$(NMe$_2$)$_6$ catalyst at 28 °C in toluene-$d_8$. These spectra are complicated by relatively slow rotation of the amide C–N bond, which leads to broadening of the N–CH$_3$ resonances (spectrum B). Evidence of carboxamide coordination to Al at this temperature is evident from comparison of the Al–N(CH$_3$)$_2$ resonances in spectra A and E. (IS = internal standard = trimethoxybenzene; S = solvent = toluene-$d_8$).
Tables of computed Cartesian coordinates (Å) and energies (hartrees) with Gibbs thermal corrections and free energies computed at 363.15 K. For transition states the value of the unique imaginary frequency is also given. Species are numbered according to the main text.

### Computed Geometrical Parameters for dimethyl amine, Figure 7

**Geometry Optimization (B3LYP/ 6-31G(d,p))**

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Computed Geometrical Parameters for dimethyltoluamide, Figure 7

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Computed Geometrical Parameters for Al dimer, Figure 7,8,9

Geometry Optimization (B3LYP/lanl2dz+d for Al, 6-31G(d,p) for H,C,N)

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Single Point (B3LYP/6-311+G(d,p) for all atoms)

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Computed Geometrical Parameters for Al-amine adduct, Figure 7

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Computed Geometrical Parameters for Al-amide adduct, Figure 7

| Geometry Optimization (B3LYP/lanl2dz+d for Al, 6-31G(d,p) for H,C,N,O) | | Total Energy (hartrees) = | -924.7512453 |
| | Gibbs Thermal Correction 363.15 K (hartrees) = | | 0.400838 |

| Single Point (B3LYP/6-311+G(d,p) for all atoms) | | Total Energy (hartress) = | -1165.433987 |

| Free Energy (sum of single point and Gibbs thermal correction) = | | -1165.033149 |

| Cartesian coordinates from optimized geometry | | | |
| Al | 1.83011 | -0.4874 | 0.00938 | H | 1.5428 | 0.32678 | 3.51072 |
| N | 1.09426 | -2.12738 | 0.39715 | O | 0.2879 | 0.42633 | -0.77594 |
| C | 1.4321 | -2.86199 | 1.60235 | C | -0.69276 | 1.14903 | -0.44373 |
| C | 0.46976 | -2.98225 | -0.59336 | C | -2.03652 | 0.52185 | -0.30718 |
| H | 0.19851 | -2.40931 | -1.48683 | C | -3.20366 | 1.10715 | -0.81947 |
| H | -0.4577 | -3.45167 | -0.21421 | C | -4.42272 | 0.44155 | -0.71972 |
| H | 1.12206 | -3.81341 | -0.92105 | C | -4.51407 | -0.8107 | -0.09702 |
| H | 0.53915 | -3.29509 | 2.09044 | C | -3.33732 | -1.39184 | 0.3986 |
| H | 2.12068 | -3.70712 | 1.41356 | C | -2.10897 | -0.74991 | 0.2829 |
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| C | 3.6422 | -1.6582 | -1.90158 | H | -3.38211 | -2.3708 | 0.86816 |
| C | 3.67577 | 0.73401 | -1.88769 | H | -1.19305 | -1.22205 | 0.63215 |
| H | 3.40224 | -1.72401 | -2.97982 | C | -5.84155 | -1.51364 | 0.04504 |
| H | 3.23086 | -2.54895 | -1.41781 | H | -6.25395 | -1.37125 | 1.05154 |
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| H | 4.78106 | 0.7396 | -1.85512 | N | -0.51946 | 2.47093 | -0.26303 |
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| N | 2.19047 | 0.54427 | 1.48895 | C | 0.79794 | 3.0498 | -0.55706 |
| C | 3.52173 | 0.99581 | 1.84595 | H | -0.91005 | 3.82523 | 1.27892 |
| C | 1.24224 | 0.79218 | 2.55328 | H | 1.50441 | 2.82231 | 0.24635 |
| H | 4.23018 | 0.75995 | 1.04676 | H | -2.2758 | 2.77506 | 0.86418 |
| H | 3.89577 | 0.52021 | 2.77196 | H | -1.83755 | 4.12782 | -0.20688 |
| H | 3.56718 | 2.088 | 2.02272 | H | 1.18193 | 2.62558 | -1.48447 |
| H | 0.25387 | 0.38659 | 2.30534 | H | 0.6811 | 4.12927 | -0.67047 |
| H | 1.11093 | 1.87184 | 2.77021 |
Computed Geometrical Parameters for piperidine, Figure 8

### Geometry Optimization (B3LYP/6-31G(d,p))

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# Computed Geometrical Parameters for N-piperidinyltoluamide, 7a, Figure 8

## Geometry Optimization (B3LYP/6-31G(d,p))
- Total Energy (hartrees) = -635.6489761
- Gibbs Thermal Correction 363.15 K (hartrees) = 0.235605

## Single Point (B3LYP/6-311+G(d,p) for all atoms)
- Total Energy (hartrees) = -635.8015873

## Free Energy (sum of single point and Gibbs thermal correction) = -635.5659823

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Computed Geometrical Parameters for $N$-piperidinylheptanamide, 7b, Figure 8

**Geometry Optimization (B3LYP/lanl2dz+d for Al, 6-31G(d,p) for H,C,N,O)**

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**Single Point (B3LYP/6-311+G(d,p) for all atoms)**

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**Free Energy (sum of single point and Gibbs thermal correction)**

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**Cartesian coordinates from optimized geometry**

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Computed Geometrical Parameters for Al adduct of 7a, Figure 8

Geometry Optimization (B3LYP/lanl2dz+d for Al, 6-31G(d,p) for H,C,N,O)

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Computed Geometrical Parameters for Al adduct of 7b, Figure 8

Geometry Optimization (B3LYP/lanl2dz+d for Al, 6-31G(d,p) for H,C,N,O)

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### Computed Geometrical Parameters for acetamide, Figure 9

#### Geometry Optimization (B3LYP/6-31G(d,p))

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### Total Energy (hartrees) = -287.8425094

**Gibbs Thermal Correction**

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**Single Point** (B3LYP/6-311+G(d,p) for all atoms)

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**Free Energy** (sum of single point and Gibbs thermal correction) = -287.8233915
Computed Geometrical Parameters for acetamide adduct, Figure 9

Geometry Optimization (B3LYP/lan12dz+d for Al, 6-31G(d,p) for H,C,N,O)

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Single Point (B3LYP/6-311+G(d,p) for all atoms)

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Cartesian coordinates from optimized geometry

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Computation Geometric Parameters for **TS1**, Figure 9

**Geometry Optimization (B3LYP/lanl2dz+d for Al, 6-31G(d,p) for H,C,N,O)**

Total Energy (hartrees) = -693.6746436

Gibbs Thermal Correction 363.15 K (hartrees) = 0.32843

Imaginary Frequency (cm\(^{-1}\)) = -156.9626

**Single Point (B3LYP/6-311+G(d,p) for all atoms)**

Total Energy (hartrees) = -934.2937093

Free Energy (sum of single point and Gibbs thermal correction) = -933.9652793

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Computed Geometrical Parameters for intermediate, 12, Figure 9

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| Free Energy (sum of single point and Gibbs thermal correction) = -933.9654775 |

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## Computed Geometrical Parameters for TS2, Figure 9

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**Single Point (B3LYP/6-311+G(d,p) for all atoms)**

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**Free Energy (sum of single point and Gibbs thermal correction)**

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