Supporting Information

Transamidation of amides with amines in solvent-free condition by CeO_2 catalyst

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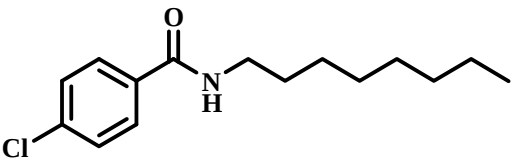
Characterization of known compounds

Products N-octyl-benzamide (Table2-1),[1] N-octyl-4-pyridinecarboxamide (Table2-8)[2], N-octyl-pyradinecarboxamide (Table2-9)[3], N-octyl-acetamide (Table2-11),[4] N-benzylhexanamide (Table3-3),[5] N-(4-methoxybenzil)-hexanamide (Table3-5),[6]1-morpholin-4-ylhexan-1-one (Table3-7)[7] and are known compounds and were identified by comparison of their NMR features with the respective reported data.

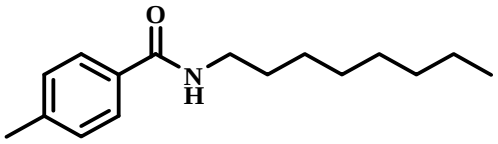
Characterization of new compounds.

N-Octyl-4-chrolobenzamide (Table2-2)



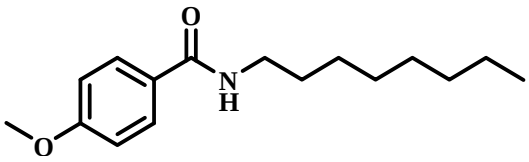
^{1}H NMR ($CDCl_3$): δ 7.72-7.68(m, 2H), 7.41-7.37(m, 2H), 6.21(br, s, 1H), 3.45-3.40(m, 2H), 1.64-1.56(m, 2H), 1.36-1.27(m, 10H), 0.88(t, J=6.9Hz, 3H)
MS: *m/z* (relative intensity) 267(M^+, 4), 139(100).

N-Octyl-4-methyl-benzlamide (Table2-3)



^{1}H NMR ($CDCl_3$): δ 7.65 (d, J=8.2Hz, 2H), 7.22(d, J=7.8Hz, 2H), 6.09(br, s, 1H), 3.46-3.41(m, 2H), 2.39(s, 3H), 1.64-1.57(m, 2H), 1.39-1.27(m, 10H), 0.88(t, J=7.1Hz, 3H)
MS: *m/z* (relative intensity) 247(M^+, 12), 119(100).

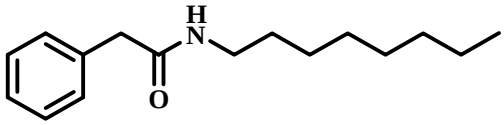
N-Octyl-4-methoxybenzamide (Table2-4)



^{1}H NMR ($CDCl_3$): δ 7.73(d, J=9.2Hz, 2H), 6.92(d, J=8.7Hz, 2H), 6.08(br, s, 1H), 3.84(s, 3H), 3.45-3.40(m, 2H), 1.64-1.56(m, 2H), 1.38-1.27(m, 10H), 0.88(t, J=7.1Hz, 3H)

MS: *m/z* (relative intensity) 263(M^+, 3), 135(100).

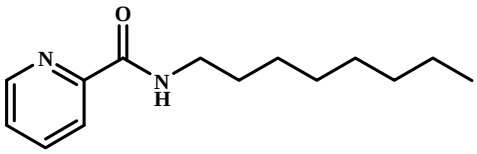
N-Octyl-benzylamide (Table2-5)



^{1}H NMR ($CDCl_3$): δ 7.35-7.24(m, 5H), 5.40(br, s, 1H), 3.56(s, 2H), 3.21-3.16(m, 2H), 1.44-1.37(m, 2H), 1.30-1.22(m, 10H), 0.87(t, J=7.1Hz, 3H)

MS: *m/z* (relative intensity) 247(M^+, 16), 92(100).

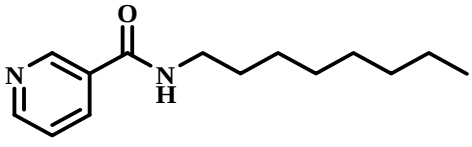
N-Octyl-2-picolinamide (Table2-6)



^{1}H NMR ($CDCl_3$): δ 8.55 (d, J=5.5Hz, 1H), 8.22-8.20(m, 1H), 8.06(br, s, 1H), 7.89-7.82(m, 1H), 7.43-7.40(m, 1H), 3.49-3.44(m, 2H), 1.66-1.60(m, 2H), 1.40-1.27(m, 10H), 0.88(t, J=6.9Hz, 3H)

MS: *m/z* (relative intensity) 234(M^+, 9), 128(100).

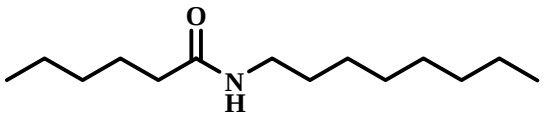
N-Octyl-nicotinamide (Table2-7)



^{1}H NMR ($CDCl_3$): δ 8.73-8.71(m, 2H), 7.61-7.60(m, 2H), 6.44(br, s, 1H), 3.48-3.43(m, 2H), 1.66-1.58(m, 2H), 1.39-1.27(m, 10H), 0.88(t, J=6.9Hz, 3H)

MS: *m/z* (relative intensity) 234(M^+, 10), 106(100).

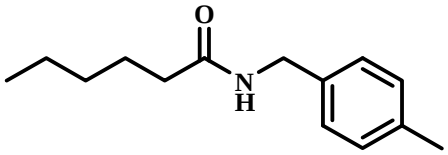
N-Octyl-hexanamide (Table2-12, 3-2)



^{1}H NMR ($CDCl_3$): δ 5.48(br, s, 1H), 3.26-3.21(m, 2H), 2.15(t, J=7.7Hz, 2H), 1.69-1.59(m, 2H), 1.50-1.45(m, 2H), 1.35-1.27(m, 14H), 0.91-0.86(m, 6H)

MS: *m/z* (relative intensity) 227(M^+, 5), 43(100).

N-(4-methoxybenzil)-hexanamide (Table3-4)



^{1}H NMR ($CDCl_3$): δ 7.18-7.13(m, 4H), 5.71(br, s, 1H), 4.40(d, J=5.5Hz, 2H), 2.33(s, 3H), 2.24-2.17(m, 2H), 1.69-1.60(m, 2H), 1.38-1.26(m, 4H), 0.92-0.87(m, 3H)

MS: *m/z* (relative intensity) 219(M^+, 16), 105(100).

Table S1 Transamidation by various metal oxides[a].

Catalyst	S_{BET} /m^2 g^{-1}	t /h	Yield (%)	V^b /mmol h^{-1} g^{-1}	V^c /mmol h^{-1} m^{-2}
CeO_2	81	0.5	21.1	42.2	0.52
TiO_2	47	1	14.3	14.3	0.30
Nb_2O_5	54	1	15.3	15.3	0.28
ZrO_2	73	1	12.9	12.9	0.18
Al_2O_3	124	1	10.3	10.3	0.08
Sc_2O_3	24	1	6.1	6.1	0.25
SiO_2	300	2	10.1	5.0	0.02
La_2O_3	18	1.5	2.4	1.6	0.09
Er_2O_3	9	1	1.6	1.6	0.18
MgO	19	2	2.2	1.1	0.06
CaO	59	2	1.5	0.8	0.01
Blank	-	1	0	-	-

[a] Reaction conditions: picolinamide (2.5 mmol), n-octylamine (5.0 mmol), metal oxide (25 mg), T = 160 ^{o}C. Yield of N-octyl picolinamide was determined by GC.

[b] Formation rate of N-octyl picolinamide per catalyst weight measured under the condition in which yield of N-octyl picolinamide was below 30%.

[c] Formation rate of N-octyl picolinamide per catalyst surface area.

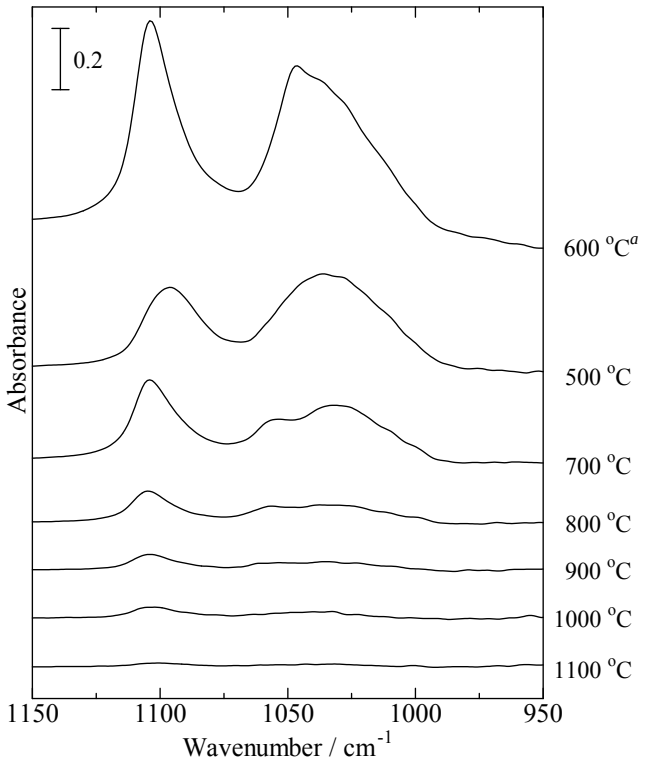


Fig. S1. Spectra of methanol complexes adsorbed to CeO_2 at different calcination temperature. Numbers in the graph are calcination temperatures ([a] JRC-CEO3).

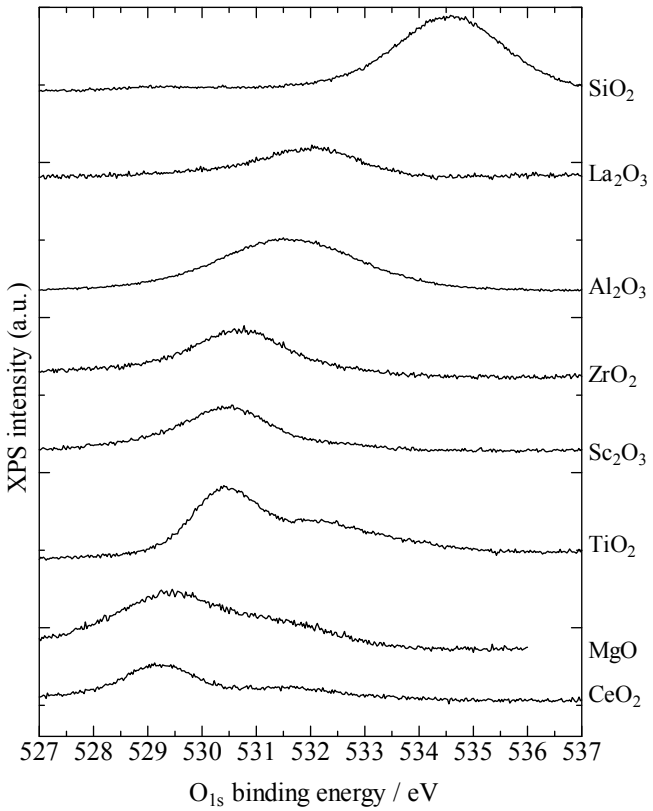


Fig. S2. XPS spectra of various metal oxides in the region of O_{1s} binding energy.

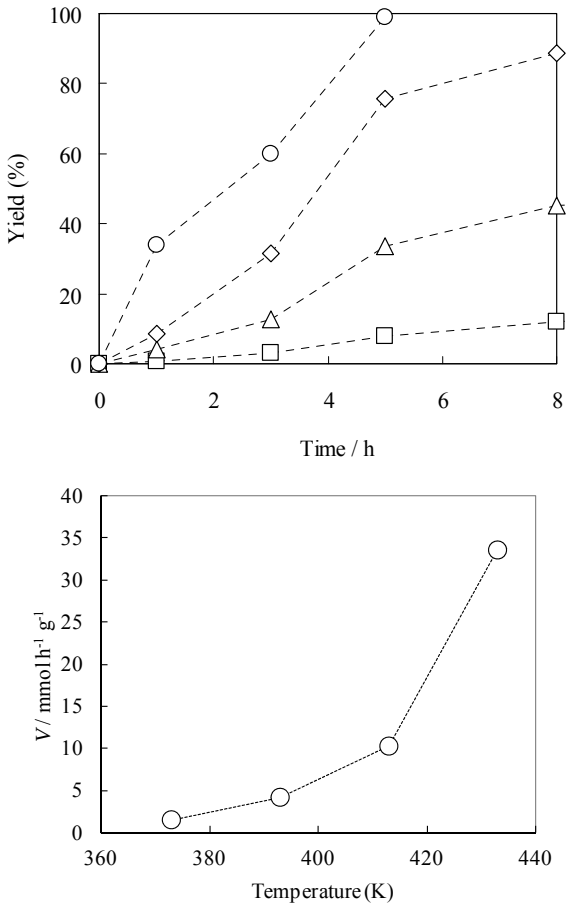


Fig. S3. Effect of reaction temperature. Conditions: picolinamide (2.5 mmol), n-octylamine (5.0 mmol), CeO_2 (25 mg).

Reference

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