ELECTRONIC SUPPLEMENTARY INFORMATION

Lewis Basic Ionic Liquids-Catalyzed Synthesis of 5-Aryl-2-oxazolidinones from Aziridines and CO₂ under Solvent-free Conditions

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1. General experimental methods:

Caution

Experiments using compressed gases CO_2 are potentially hazardous and must only be carried out by using the appropriate equipment and under rigorous safety precautions.

Materials

Aziridines and ILs were synthesized according to the published procedures.^{1, 2} CO_2 with a purity of 99.99% was commercially available. The other organic and inorganic compounds from Tianjin Guangfu Fine Chemical Research Institute were used without further purification except for the solvents, which were distilled by the known method prior to use.

Experimental methods

1H NMR spectra was recorded at Bruck 300 or 400 spectrometer in CDCl3 and TMS (0 ppm) was used as internal reference, 13C NMR was recorded at 75 or 100.6 MHz in CDCl3 and CDCl3 (77.0 ppm) was used as internal reference. ESI-MS were recorded on a Thermo Finnigan LCQ Advantage spectrometer in ESI mode with a spray voltage of 4.8 kV. GC analyses were performed on Shimadzu GC-2014, equipped with a capillary column (RTX-5, 30 m \times 0.25 µm) using a flame ionization detector. Melting points were measured on an X4 apparatus and uncorrected. In situ FTIR was collected on a Mettler Toledo React IR ic10 analysis system. Melting points were measured on an X4 apparatus and uncorrected.

2. General procedures for the preparation of ionic liquids:

[C₄DABCO]Br:

A solution of freshly sublimed DABCO (0.5609 g, 5 mmol) in MeCN (5 mL) was prepared at r.t. under Ar in a flame dried round-bottomed flask equipped with a reflux condenser. The resulting clear, colorless solution was treated with 1-bromobutane (0.269 mL, 2.5 mmol), added dropwise via syringe, and the reaction mixture was heated to 80 °C (oil bath temperature) and stirred for 22 h. After being cooled to r.t., the reaction mixture was transferred via cannula into 20 mL of Et_2O , yielding a white slurry which eventually separated into two layers. The whole was transferred to a separatory funnel, and the bottom layer was collected, washed repeatedly with Et_2O and dried under high vacuum at 60 °C for 16 h to yield 1-butyl-4-aza-1-azaniabicyclo[2.2.2]octane bromide as a white glassy solid.

[C₄DABCO]Cl:

According to the synthetic procedure of $[C_4DABCO]Br$, 1-butyl-4-aza-1-azaniabicyclo[2.2.2] octane chloride was yielded as a white glassy solid.

[C₄DABCO]OH:

Solid potassium hydroxide (0.112 g, 2 mmol) was added to a solution of $[C_4DABCO]Br$ (0.4984 g, 2 mmol) in dry methylene chloride (2 mL), and the mixture was stirred vigorously at r.t. for 10 h. The precipitated KBr was filtered off, and the filtrate was evaporated to leave the crude $[C_4DABCO]OH$ as a white solid that was washed with ether (2 × 2 mL) and dried at 90 °C for 10 h to prepare the pure ionic liquid 1-butyl-4-aza-1-azaniabicyclo[2.2.2]octane hydroxide.

[C₈DABCO]Br:

According to the synthetic procedure of $[C_4DABCO]Br$, 1-octyl-4-aza-1-azaniabicyclo[2.2.2] octane bromide was yielded as a yellow glassy solid.

[C₈DABCO]BF₄:

A solution of 1-octyl-4-aza-1-azaniabicyclo[2.2.2]octane bromide (0.4972 g, 1.63 mmol) in MeCN (1.0 mL), prepared at r.t. under Ar in a flame-dried round-bottomed flask, was transferred via cannula to a slurry of NaBF₄ (0.181 g, 1.65 mmol) in MeCN (1.5 mL). A 0.5 mL MeCN rinse was used to ensure complete transfer. A white precipitate formed immediately and the resulting slurry was stirred at r.t. for 24 h. Filtration followed by concentration of the filtrate in vacuo yielded a colorless, viscous liquid shown to be contaminated with bromide by a positive AgNO₃ test. The crude was partitioned between CH₂Cl₂ and H₂O, and the CH₂Cl₂ layer was washed repeatedly with H₂O until the aqueous layer gave a negative AgNO₃ test. The CH₂Cl₂ extract was dried (Na₂SO₄), subjected to filtration and concentrated in vacuo. Drying under high vacuum at 60 °C for 3 d yielded 1-octyl-4-aza-1-azaniabicyclo[2.2.2]octane tetrafluoroborate as a clear colourless liquid.

[C₈DABCO]NTf₂:

A solution of LiN(SO₂CF₃)₂ (0.465 g, 1.62 mmol) in MeCN (1.0 mL), prepared at r.t. under Ar in a flame-dried round-bottomed flask, was transferred via cannula to a solution of 1-octyl-4-aza-1-azaniabicyclo[2.2.2]octane bromide (0.488 g, 1.60 mmol) in MeCN (1.5 mL). A 0.5 mL MeCN rinse was used to ensure complete transfer. A white precipitate formed within 5 min and the resulting slurry was stirred at r.t. for 47 h. Filtration followed by concentration of the filtrate in vacuo yielded a colorless liquid shown to be contaminated with chloride by a positive AgNO₃ test. The crude was partitioned between CH₂Cl₂ and H₂O, and the CH₂Cl₂ layer was washed repeatedly with H₂O until the aqueous layer gave a negative AgNO₃ test. The CH₂Cl₂ extract was dried (Na₂SO₄), subjected to filtration and concentrated in vacuo. Drying under high vacuum at 60 °C for 5 d yielded 1-octyl-4-aza-1-azaniabicyclo[2.2.2]octane bis(trifluoromethylsulfonyl)imide as a colorless liquid.

[C₈DABCO]PF₆:

A solution of 1-octyl-4-aza-1-azaniabicyclo[2.2.2]octane bromide (0.4911 g, 1.61 mmol) in MeCN (1.0 mL), prepared at r.t. under Ar in a flame-dried round-bottomed flask, was transferred via cannula to a slurry of KPF₆ (0.3018 g, 1.64 mmol) in MeCN (1.0 mL). A 0.5 mL MeCN rinse was used to ensure complete transfer. A white precipitate formed immediately and the resulting slurry was stirred at r.t. for 20 h. Filtration followed by concentration of the filtrate in vacuo yielded an oily, white solid shown to be contaminated with bromide by a positive AgNO₃ test. The crude was partitioned between CH_2Cl_2 and H_2O , and the CH_2Cl_2 layer was washed repeatedly with H_2O until the aqueous layer gave a negative AgNO₃ test. The CH₂Cl₂ extract was dried (Na₂SO₄), subjected to filtration and concentrated in vacuo. Drying under high vacuum at 60 °C for 5 d yielded 1-octyl-4-aza-1-azaniabicyclo[2.2.2]octane hexafluorophosphate as a white solid.

[C₁₂DABCO]Br:

According to the synthetic procedure of $[C_4DABCO]Br$, 1-dodecyl-4-aza-1-azaniabicyclo[2.2.2]octane bromide was yielded as a yellow glassy solid.

[C₄MIm]Br:

Under N_2 , freshly dried 1-methylimidazole (1.6 mL, 20 mmol) and 1-bromobutane (3.7 mL, 34.4 mmol) were added to dry toluene (2 mL) in a round-bottomed Schlenk flask. The mixture was heated under reflux under N_2 for 24 h, upon which two layers had formed. The flask was allowed to cool to room temperature and was then cooled to -10 °C overnight, during which time a white solid was formed. The excess toluene was decanted, while N_2 was being passed over the product layer. The resulting white precipitate was washed with dry diethyl ether and then dried in vacuo for 24 h to afford 1-butyl-3-methylimidazolium bromide as a light yellow liquid.

[C₄MIm]BF₄:

To a solution of $[C_4MIm]Br$ (2.1912 g, 10 mmol) in acetone (10 mL) at room temperature was added sodium tetrafluoroborate (1.0979 g, 10 mmol). Afer 24 h stirring, the reaction mixture was filtered and the volatiles were removed under reduced pressure. Drying in vacuo for 10 h afforded 1-butyl-3-methylimidazolium tetrafluoroborate as a light yellow liquid.

[C₈MIm]Br:

According to the synthetic procedure of $[C_4MIm]Br$, 1-octyl-3-methylimidazolium bromide was yielded as a colourless liquid.

[C₈MIm]BF₄:

According to the synthetic procedure of $[C_4MIm]BF_4$, 1-octyl-3-methylimidazolium tetrafluoroborate was yielded as a white glassy solid.

3. General procedure for the preparation of aziridines



Typical procedure was described as below. The bromine (32.0 g, 0.2 mol) in dry CH_2Cl_2 (40 mL) was added dropwise over 30 min to ice-cooled 40 mL CH_2Cl_2 solution of dimethyl sulfide (12.4 g, 0.2 mol). During the addition, light orange crystals of bromodimethyl sulfonium bromide began to separate. After

addition of bromine, the orange crystals S1 were collected by filtration and then washed with dry diethyl ether and dried under vacuum. Yield: 80%, Mp 80 °C (dec).

Olefin (160 mmol) was added dropwise to the 160 mL CH₃CN solution of **S1** (35.56 g, 160 mmol) in ice-water bath. During the addition, the white solid began to separate. The solution was further stirred for 10 min. The crystals **S2** was collected by filtration, dried under vacuum. Yield: 32-38.6 %.

A solution of amine (20-50 mmol) in water was added dropwise to a stirred solution of compound S2 (10 mmol) in 20 mL of H₂O at r.t., and the resulting mixture was stirred overnight. The mixture was added into 20 mL of saturated brine, extracted with diethyl ether (3×20 mL), dried with anhydrous MgSO₄ overnight and evaporated under reduced pressure. Aziridine was obtained by distillation under reduced pressure. Yield: 85-100 %.

4. General Procedure for Carboxylation of Aziridine with CO₂

In a typical reaction, the carboxylation of aziridines with CO_2 was carried out in a 25 mL stainless steel autoclave. Aziridine (1 mmol) were charged into the reactor at room temperature. CO_2 was introduced into the autoclave and then the mixture was stirred at predetermined temperature for 15 min to reach the equilibration. The pressure was then adjusted to the desired pressure and the mixture was stirred continuously. When the reaction finished, the reactor was cooled in ice-water and CO_2 was ejected slowly. An aliquot of sample was taken from the resultant mixture and dissolved in dry CH_2Cl_2 for GC analysis (GC analyses were performed on Shimadzu GC-2014, equipped with a capillary column (RTX-5, 30 m × 0.25 μ m×0.25 μ m) using a flame ionization detector. The residue was purified by column chromatography on silica gel (eluting with 8:1 to 1:1 petroleum ether/ethyl acetate) to afford the product. The products were further identified by ¹H NMR, ¹³C NMR and MS which are consistent with those reported in the literature^{1,3} and in good agreement with the assigned structures.

5. Characterization of ionic liquids

[C₄DABCO]Br:

White glassy solid; Mp 36-37 °C; ¹H NMR (300 MHz, CDCl₃) δ 3.65 (t, ³*J* = 7.2 Hz, 6 H), 3.47 (t, ³*J* = 8.4 Hz, 2 H), 3.22 (t, ³*J* = 6.6 Hz, 6 H), 1.70-1.75 (m, 2 H), 1.36-1.40 (m, 2 H), 0.94 (t, ³*J* = 7.2 Hz, 3 H); ¹³C {¹H} NMR (75 MHz, CDCl₃) δ 64.3, 52.4, 45.4, 23.9, 19.7, 13.6; ESI-MS calcd for C₁₀H₂₁N₂Br 249.19, found 169.38 [M-Br]⁺, 79.02 [M-C₁₀H₂₁N₂]⁻.

[C₄DABCO]OH:

White solid; Mp 45-46 °C; ¹H NMR (400 MHz, D₂O) δ 3.39 (t, ³*J* = 7.6 Hz, 6 H), 3.25 (t, ³*J* = 8.8 Hz, 2 H), 3.19 (t, ³*J* = 7.2 Hz, 6 H), 1.74 (quintet, ³*J* = 8 Hz, 2 H), 1.33-1.42 (m, 2 H), 0.94 (t, ³*J* = 7.6 Hz, 3 H); ¹³C {¹H} NMR (100.6 MHz, D₂O) δ 64.4, 52.0, 44.1, 23.1, 19.1, 12.7; ESI-MS calcd for C₁₀H₂₂N₂O 186.29, found 169.3 [M-OH]⁺, bromide was not tested under the negative ion mode.

[C₄DABCO]Cl:

White glassy solid; Mp 36-37 °C; ¹H NMR (400 MHz, CDCl₃) δ 3.67 (t, ³*J* = 7.2 Hz, 6 H), 3.54 (t, ³*J* = 8.4 Hz, 2 H), 3.25 (t, ³*J* =,7.2 Hz, 6 H), 1.69-1.77 (m, 2 H), 1.36-1.45 (m, 2 H), 0.97 (t, ³*J* =7.2 Hz, 3 H); ¹³C {¹H} NMR (100.6 MHz, CDCl₃) δ 64.3, 52.4, 45.4, 23.9, 19.7, 13.7; ESI-MS calcd for C₁₀H₂₁N₂Cl 204.74, found 169.44 [M-Cl]⁺.

[C₈DABCO]Br:

Yellow glassy solid; Mp 37-38 °C; ¹H NMR (400 MHz, CDCl₃) δ 3.49 (t, ³*J* = 7.6 Hz, 6 H), 3.27 (t, ³*J* = 8.4 Hz, 2 H), 3.08 (t, ³*J* = 7.2 Hz, 6 H), 1.59 (s, 2 H), 1.06-1.15 (m, 10 H), 0.68 (t, ³*J* = 7.2 Hz, 3 H); ¹³C {¹H} NMR (100.6 MHz, CDCl₃) δ 64.1, 52.0, 45.0, 31.1, 28.6, 28.5, 25.9,22.1, 21.6, 13.6; ESI-MS calcd for C₁₄H₂₉N₂Br 305.3, found 225.46 [M-Br]⁺, 79.03 [M-C₁₄H₂₉N₂]⁻.

[C₈DABCO]BF₄:

White glassy solid; Mp 37-38 °C; ¹H NMR (400 MHz,CDCl₃) δ 3.28 (t, ³*J* = 7.6 Hz, 6 H), 3.10-3.16 (m, 8 H), 1.66 (s, 2 H), 1.20-1.27 (m, 10 H), 0.81 (t, ³*J* = 7.2 Hz, 3 H); ¹³C {¹H} NMR (100.6 MHz, CDCl₃) δ 64.5, 52.0, 44.9, 31.3, 28.7, 26.0, 22.2, 21.4, 13.7; ¹⁹F {¹H} NMR (377 MHz, CDCl₃) δ -151.10, -151.15; ESI-MS calcd for C₁₄H₂₉N₂BF₄ 312.2, found 225.45 [M-BF₄]⁺, 87.1 [M-C₁₄H₂₉N₂]⁻.

[C₈DABCO]PF₆:

White solid; Mp 161-163 °C; ¹H NMR (400 MHz, CDCl₃) δ 3.27-3.30 (m, 6 H), 3.13-3.22 (m, 8 H), 1.70 (s, 2 H), 1.26-1.33 (m, 10 H), 0.87 (t, ³J = 7.2 Hz, 3 H); ¹³C {¹H} NMR (100.6 MHz, CDCl₃) δ 65.0, 52.5, 45.2, 31.6, 28.94, 28.92, 26.2, 22.5, 21.7, 14.0; ¹⁹F {¹H} NMR (377 MHz, CDCl₃) δ -71.02, -72.91; ³¹P {¹H} NMR

(161.9 MHz, CDCl₃) δ -144.33 (septet, $J_{P,F}$ = 712Hz); ESI-MS calcd for C₁₄H₂₉N₂PF₆ 370.36, found 225.43 [M-PF₆]⁺, 145.20 [M-C₁₄H₂₉N₂]⁻.

[C₈DABCO]NTf₂:

Colorless liquid; ¹H NMR (400 MHz, CDCl₃) δ 3.17 (t, ³*J* = 6.4 Hz, 6 H), 2.98-3.07 (m, 8 H), 1.58 (s, 2 H), 1.16-1.21 (m, 10 H), 0.76 (t, ³*J* = 6.8 Hz, 3 H); ¹³C {¹H} NMR (100.6 MHz, CDCl₃) δ 117.2 (q, *J*_{C,F} = 321 Hz), 62.4, 49.9, 42.5, 28.9, 26.3, 26.2, 23.5, 19.9, 19.0, 11.4; ¹⁹F {¹H} NMR (377 MHz, CDCl₃) δ -81.60; ESI-MS calcd for C₁₆H₂₉N₃O₄S₂F₆ 505.54, found 225.43 [M-C₂F₆NO₄S₂]⁺, 280.10 [M-C₁₄H₂₉N₂]⁻.

[C₁₂DABCO]Br:

White solid; Mp 59-60 °C; ¹H NMR (400 MHz,CDCl₃) δ 3.64 (s, 6 H), 3.46 (t, ³*J* = 7.6 Hz, 2 H), 3.24 (s, 6 H), 1.21-1.30 (m, 20 H), 0.84 (t, ³*J* = 5.2 Hz, 3 H); ¹³C {¹H} NMR (100.6 MHz, CDCl₃) δ 64.5, 52.4, 45.3, 31.8, 29.5, 29.4, 29.3, 29.2, 29.1, 26.3, 22.6, 22.1, 14.0; ESI-MS calcd for C₁₈H₇N₂Br 338.22, found 281.82 [M-Br]⁺, 79.03 [M-C₁₈H₃₇N₂]⁻.

[C₄MIm]Br:

Light yellow liquid; ¹H NMR (400 MHz, CDCl₃) δ 10.27 (s, 1 H), 7.60 (t, ³*J* = 1.6 Hz, 1 H), 7.47 (t, ³*J* = 1.6 Hz, 1 H), 4.28 (t, ³*J* = 7.2 Hz, 2 H), 4.07 (s, 3 H), 1.85 (quintet, ³*J* = 7.6 Hz, 2 H), 1.32 (sextet, ³*J* = 7.6 Hz, 2 H), 0.89 (t, ³*J* = 7.6 Hz, 3 H); ¹³C {¹H} NMR (100.6 MHz, D₂O) δ 135.8, 123.2, 122.2, 49.3, 35.7, 31.3, 18.7, 12.6; ESI-MS calcd for C₈H₁₅N₂Br 219.12, found 139.32 [M-Br]⁺, 79.03 [M-C₈H₁₅N₂]⁻.

[C₄MIm]BF₄:

Light yellow liquid; ¹H NMR (400 MHz, D₂O) δ 8.71 (s, 1 H), 7.51 (s, 1 H), 7.47 (s, 1 H), 4.22-4.23 (m, 2 H), 3.94 (s, 3 H), 1.87-1.89 (m, 2 H), 1.35-1.37 (m, 2 H), 0.96 (t, ³*J* = 7.6 Hz, 3 H); ¹³C {¹H} NMR (100.6 MHz, D₂O) δ 135.9, 123.5, 122.2, 49.3, 35.6, 31.3, 18.8, 12.7; ¹⁹F {¹H} NMR (377 MHz, CDCl₃) δ -150.12, -150.30; ESI-MS calcd for C₈H₁₅N₂BF₄ 226.02, found 139.32 [M-BF₄]⁺, 87.11 [M-C₈H₁₅N₂]⁻.

[C₈MIm]Br:

Colourless liquid; ¹H NMR (400 MHz, CDCl₃) δ 10.06 (s, 1 H), 7.59 (s, 1 H), 7.40 (s, 1 H), 4.17 (t, ³*J* = 6.8 Hz, 2 H), 3.99 (s, 3 H), 1.76-1.77 (m, 2 H), 1.09-1.17 (m, 10 H), 0.70 (t, ³*J* = 6.4Hz, 3 H); ¹³C {¹H} NMR (100.6 MHz, CDCl₃) δ 136.0, 123.1, 121.4, 49.2, 35.9, 30.7, 29.4, 28.1, 28.0, 25.3, 21.6, 13.2; ESI-MS calcd for C₁₂H₂₃N₂Br 275.23, found 195.46 [M-Br]⁺, 79.03 [M-C₁₂H₂₃N₂]⁻.

[C₈MIm]BF₄:

Light yellow liquid; ¹H NMR (400 MHz, CDCl₃) δ 8.70 (s, 1 H), 7.38 (s, 1 H), 7.32 (s, 1 H), 4.12 (t, ³*J* = 7.2 Hz, 2 H), 3.89 (s, 3 H), 1.82 (t, ³*J* = 6.8 Hz, 2 H), 1.20-1.26 (m, 10 H), 0.81 (t, ³*J* = 6.8 Hz, 3 H); ¹³C {¹H} NMR (100.6 MHz, CDCl₃) δ 136.0, 123.7, 122.1, 49.9, 36.0, 31.5, 29.9, 28.9, 28.7, 26.0, 22.4, 13.9; ¹⁹F {¹H} NMR (377 MHz, CDCl₃) δ -150.99, -151.05; ESI-MS calcd for C₁₂H₂₃N₂BF₄ 282.13, found 195.39 [M-BF₄]⁺, 87.10 [M-C₁₂H₂₃N₂]⁻.

6. Characterization of aziridines

2-Phenylaziridine:

¹H NMR (400 MHz, CDCl₃) δ 0.81 (s, 1H), 1.79 (d, ²J = 3.2 Hz, 1H), 2.20 (d, ²J = 6.0 Hz, 1H), 3.01 (dd, ³J = 3.6 Hz, ³J = 2.4 Hz, 1H), 7.21-7.32 (m, 5H); ESI-MS calcd for C₈H₉N 119.07, found 120.26 [M + H]⁺.

1-Methyl-2-phenylaziridine:

¹H NMR (400 MHz, CDCl₃) δ 1.62 (d, ²*J* = 6.4 Hz, 1H), 1.90 (d, ²*J* = 3.2 Hz, 1H), 2.26 (dd, ³*J* = 3.2 Hz, ³*J* = 3.2 Hz, 1H), 2.48 (s, 3H), 7.19-7.30 (m,5H); ESI-MS calcd for C₉H₁₁N 133.19, found 134.21 [M + H]⁺.

1-Ethyl-2-phenylaziridine:

¹H NMR (400 MHz, CDCl₃) δ 1.17 (t, ³*J* = 9.6 Hz, 3H), 1.65 (d, ²*J* = 8.8 Hz, 1H), 1.89 (d, ²*J* = 4.4 Hz, 1H), 2.30 (dd, ³*J* = 4.4 Hz, ³*J* = 4.8 Hz, 1H), 2.44 (q, ³*J* = 9.6 Hz, 2H), 7.18-7.31 (m, 5H); ESI-MS calcd for C₁₀H₁₃N 147.10, found 148.31 [M + H]⁺.

1-Propyl-2-phenylaziridine:

¹H NMR (400 MHz, CDCl₃) δ 0.95 (t, ³J = 10.0 Hz, 3H), 1.60-1.67 (m, 3H), 1.89 (d, ²J = 4.0 Hz, 1H), 2.24-2.33 (m, 2H), 2.43-2.51 (m, 1H), 7.18-7.31 (m, 5H); ESI-MS calcd for C₁₁H₁₅N 161.12, found 162.28 [M + H]⁺.

1-Isopropyl-2-phenylaziridine:

¹H NMR (300 MHz, CDCl₃) δ 1.17 (d, ³*J* = 0.9 Hz, 3H), 1.19 (d, ³*J* = 0.9 Hz, 3H), 1.57-1.66 (m, 2H), 1.89 (d, ²*J* = 3.3 Hz, 1H), 2.34 (dd, ³*J* = 3.3 Hz, ³*J* = 3.3 Hz, 1H), 7.17-7.31 (m, 5H); ESI-MS calcd for C₁₁H₁₅N 161.12, found 162.32 [M + H]⁺.

1-Cyclopropyl-2-phenylaziridine:

¹H NMR (300 MHz, CDCl₃) δ 0.41-0.50 (m, 2H), 0.55-0.67 (m, 2H), 1.60-1.67 (m, 1H), 1.86-1.88 (m, 2H), 2.57 (dd, ³J = 3.6 Hz, ³J = 3.0 Hz, 1H), 7.17-7.30 (m, 5H); ESI-MS calcd for C₁₁H₁₃N 159.10, found 160.32 [M + H]⁺.

1-Butyl-2-phenylaziridine:

¹H NMR (300 MHz, CDCl₃) δ 0.91 (t, ³*J* = 7.2 Hz, 3H), 1.33-1.45 (m, 2H), 1.55-1.67 (m, 3H), 1.88 (d, ²*J* = 3.3 Hz, 1H), 2.27-2.36 (m, 2H), 2.45-2.54 (m, 1H), 7.17-7.31 (m, 5H); ESI-MS calcd for C₁₂H₁₇N 175.14, found 176.38 [M + H]⁺.

1-Isobutyl-2-phenylaziridine:

¹H NMR (300 MHz, CDCl₃) δ 0.95 (d, ³*J* = 6.6 Hz, 3H), 0.98 (d, ³*J* = 6.6 Hz, 3H), 1.65 (d, ²*J* = 6.3 Hz, 1H), 1.85-1.94 (m, 2H), 2.08 (dd, ³*J* = 6.3 Hz, ³*J* = 6.6 Hz, 1H), 2.28 (q, ³*J* = 3.3 Hz, 1H), 2.44 (dd, ³*J* = 7.2 Hz, ²*J* = 11.4 Hz, 1H), 7.17-7.31 (m, 5H); ESI-MS calcd for C₁₂H₁₇N 175.14, found 176.36 [M + H]⁺.

1-Tert-butyl-2-phenylaziridine:

¹H NMR (300 MHz, CDCl₃) δ 1.05 (s, 9H), 1.64 (dd, ²*J* = 3.0 Hz, ³*J* = 0.9 Hz, 1H), 1.89 (dd, ²*J* = 6.3 Hz, ³*J* = 0.6 Hz, 1H), 2.62 (q, ³*J* = 3.0 Hz, 1H), 7.16-7.33 (m, 5H); ESI-MS calcd for C₁₂H₁₇N 175.14, found 176.19 [M + H]⁺.

1-Benzyl-2-phenylaziridine:

¹H NMR (300 MHz, CDCl₃) δ 1.84 (d, ²*J* = 6.3 Hz, 1H), 1.98 (d, ²*J* = 3.3 Hz, 1H), 2.50 (q, ³*J* = 3.3 Hz, 1H), 3.65 (ABq, ³*J*_{AB} = 13.8 Hz, Δv_{AB} = 18.8 Hz, 2H), 7.18-7.38 (m, 10H); ESI-MS calcd for C₁₅H₁₅N 209.29, found 210.13 [M + H]⁺.

1-Cyclohexyl-2-phenylaziridine:

¹H NMR (300 MHz, CDCl₃) δ 1.19-1.87 (m, 13H), 2.34 (dd, ³*J* =3.3 Hz, ³*J* =3.0 Hz, 1H), 7.17-7.27 (m, 5H); ESI-MS calcd for C₁₄H₁₉N 201.15, found 202.37 [M + H]⁺.

2-(4-Chlorophenyl)-1-ethylaziridine:

¹H NMR (300 MHz, CDCl₃) δ 1.18 (t, ³*J* = 6.9 Hz, 3H), 1.65 (d, ²*J* = 6.6 Hz, 1H), 1.83 (d, ²*J* = 3.3 Hz, 1H), 2.25-2.46 (m, 3H), 7.15-7.23 (m, 4H); ESI-MS calcd for C₁₀H₁₂NCl 181.66, found 182.13 [M + H]⁺.

2-(4-Methylphenyl)-1-ethylaziridine:

¹H NMR (400 MHz, CDCl₃) δ 1.19 (t, ³*J* = 7.2 Hz, 3H), 1.62 (d, ²*J* = 6.4 Hz, 1H), 1.86 (d, ²*J* = 3.2 Hz, 1H), 2.26 (dd, ³*J* = 3.6 Hz, ³*J* = 3.2 Hz, 1H), 2.31 (s, 3H), 2.37-2.48 (m, 2H), 7.09-7.15 (m, 4H); ESI-MS calcd for C₁₁H₁₅N 161.24, found 162.20 [M + H]⁺.

7. Characterization of oxazolidinones

5-Phenyloxazolidin-2-one:

White crystals; ¹H NMR (300 MHz, CDCl₃) δ 3.55 (t, ³*J* = 8.4 Hz, 1H), 3.99 (t, ³*J* = 8.4 Hz, 1H), 5.62 (t, ³*J* = 8.4 Hz, 1H), 6.08 (brs, 1H), 7.35-7.43 (m, 5H); ¹³C NMR (75 MHz, CDCl₃) δ 48.2, 77.8, 125.6, 128.9, 138.4, 160.1; ESI-MS calcd for C₉H₉NO₂ 163.06, found 164.18 (M + H)⁺, 186.28 (M + Na)⁺, 349.03 (2M + Na)⁺.

3-Methyl-5-phenyloxazolidin-2-one:

White crystals; ¹H NMR (300 MHz, CDCl₃) δ 2.89 (s, 3H), 3.42 (t, ³*J*=8.4 Hz, 1H), 3.90 (t, ³*J*=8.4 Hz, 1H), 5.45 (t, ³*J*=8.0 Hz, 1H), 7.33-7.38 (m, 5H); ¹³C NMR (75 MHz, CDCl₃) δ 30.7, 54.0, 73.0, 125.3, 128.5, 128.6, 138.4, 157.9; ESI-MS calcd for C₁₀H₁₁NO₂ 177.08, found 178.21 (M + H)⁺, 200.25 (M + Na)⁺, 377.00 (2M + Na)⁺.

3-Ethyl-5-phenyloxazolidin-2-one:

Colorless liquid; ¹H NMR (300 MHz, CDCl₃) δ 1.17 (t, ³*J* = 7.2 Hz, 3H), 3.29-3.45 (m, 3H), 3.92 (t, ³*J* = 8.7 Hz, 1H), 5.48 (t, ³*J* = 7.8 Hz, 1H), 7.34-7.42 (m, 5H); ¹³C NMR (75 MHz, CDCl₃) δ 12.4, 38.8, 51.5, 74.2, 125.4, 128.6, 128.8, 138.8, 157.5; ESI-MS calcd for C₁₁H₁₃NO₂ 191.09, found 192.29 (M + H)⁺, 214.38 (M + Na)⁺, 405.01 (2 M + Na)⁺.

3-Ethyl-4-phenyloxazolidin-2-one:

Colorless liquid; ¹H NMR (400 MHz, CDCl₃) δ 1.05 (t, ³J = 7.2 Hz, 3H), 2.79-2.88 (m, 1H), 3.48-3.57 (m, 1H), 4.10 (t, ³J = 8.0 Hz, 1H), 4.62 (t, ³J = 8.8 Hz, 1H), 4.81 (t, ³J = 7.2 Hz, 1H), 7.30 7.44 (m, 5H); ¹³C NMR (75 MHz, CDCl₃) δ 12.1, 36.8, 59.3, 69.7, 126.9, 129.0, 129.2, 137.8, 158.1; ESI-MS calcd for C₁₁H₁₃NO₂ 191.09, found 192.29 (M + H)⁺, 214.38 (M + Na)⁺, 405.01 (2M + Na)⁺.

1, 4-Diethyl-2, 5-diphenylpiperazine:

White crystals; ¹H NMR (400 MHz, CDCl₃) δ 0.91 (t, ³*J*=7.2 Hz, 6H), 1.99-2.05 (m, 2H), 2.30 (t, ³*J*=10.8 Hz, 2H), 2.54-2.62 (m, 2H), 3.08 (dd, ²*J*=11.6 Hz, ³*J*=2.4 Hz, 2H), 3.45 (dd, ³*J*=2.0 Hz, ²*J*=12.0 Hz, 2H), 7.29-7.43 (m, 10H). LC-MS, calcd for C₂₀H₂₆N₂ 294.21, found 295.35 (M + H)⁺.

1, 4-Diethyl-2, 3-diphenyl-piperazine:

Colorless liquid; ¹H NMR (400 MHz, CDCl₃) δ 1.01 (t, ³*J*=7.2 Hz, 6H), 2.17-2.26 (m, 2H), 2.33-2.26 (m, 2H), 2.65-2.69 (m, 2H), 2.95-2.99 (q, ³*J*=6.0 Hz, 2H), 3.73 (s, 2H), 7.27-7.38 (m, 6H), 7.69-7.71 (d, ³*J*=7.2 Hz, 4H). LC-MS, calcd for C₂₀H₂₆N₂ 294.21, found 295.31(M+H)⁺.

3-Propyl-5-phenyloxazolidin-2-one:

Colorless liquid; ¹H NMR (300 MHz, CDCl₃) δ 0.91 (t, ³*J*=7.2 Hz, 3H), 1.52-1.61 (m, 2H), 3.18-3.31 (m, 2H) 3.40 (t, ³*J*=8.0 Hz, 1H), 3.90 (t, ³*J*=8.8 Hz, 1H), 5.46 (t, ³*J*=8.0 Hz, 1H), 7.31-7.37 (m, 5H); ¹³C NMR (75 MHz, CDCl₃) δ 10.7, 20.3, 45.5, 51.8, 74.0, 125.2, 128.4, 128.5, 138.7, 157.6; ESI-MS calcd for C₁₂H₁₅NO₂ 205.11, found 206.30 (M + H)⁺, 228.30 (M + Na)⁺, 433.04 (2M + Na)⁺.

3-Isopropyl-5-phenyloxazolidin-2-one:

Colorless liquid; ¹H NMR (300 MHz, CDCl₃) δ 1.16 (d, ³*J*=6.8 Hz, 3H), 1.22 (d, ³*J*=6.8 Hz, 3H), 3.37 (t, ³*J*=8.0 Hz, 1H), 3.87 (t, ³*J*=8.8 Hz, 1H), 4.13-4.23 (m, 1H), 5.48 (t, ³*J*=8.0 Hz, 1H), 7.34-7.42 (m, 5H); ¹³C NMR (75 MHz, CDCl₃) δ 19.1, 19.6, 44.5, 47.0, 74.2, 125.1, 128.3, 128.5, 138.7, 156.7; ESI-MS calcd for C₁₂H₁₅NO₂ 205.11, found 206.29 (M + H)⁺, 433.08 (2M + Na)⁺.

3-Cyclopropyl-5-phenyloxazolidin-2-one:

White crystals; ¹H NMR (300 MHz, CDCl₃) δ 0.75 (s, 4H), 2.55-2.59 (m, 1H), 3.43 (t, ³*J*=8.1 Hz, 1H), 3.88 (t, ³*J*=8.7 Hz, 1H), 5.42 (t, ³*J*=8.1 Hz, 1H), 7.28-7.37 (m, 5H); ¹³C NMR (75 MHz, CDCl₃) δ 5.4, 5.8, 25.7, 53.3, 74.3, 125.4, 128.6, 128.7, 138.5, 157.9; ESI-MS calcd for C₁₂H₁₃NO₂ 203.09, found 429.27 (2M + Na)⁺, 631.80 (3M + Na)⁺.

3-Butyl-5-phenyloxazolidin-2-one:

Colorless liquid; ¹H NMR (300 MHz, CDCl₃) δ 0.94 (t, ³*J*=7.2 Hz, 3H), 1.31-140 (m, 2H), 1.51-1.58 (m, 2H), 3.23-3.38 (m, 2H) 3.43 (t, ³*J*=8.0 Hz, 1H), 3.92 (t, ³*J*=8.8 Hz, 1H), 5.49 (t, ³*J*=8.0 Hz, 1H), 7.28-7.42 (m, 5H); ¹³C NMR (75 MHz, CDCl₃) δ 13.4, 19.5, 29.1, 43.6, 51.8, 74.1, 125.2, 128.4, 128.5, 138.7, 157.7; ESI-MS calcd for C₁₃H₁₇NO₂ 219.13, found 220.34 (M + H)⁺, 259.48 (M + K)⁺, 461.05 (2M + Na)⁺.

3-Isobutyl-5-phenyloxazolidin-2-one:

White crystals; ¹H NMR (300 MHz, CDCl₃) δ 0.91 (d, ³*J*=4.8 Hz, 3H), 0.93 (d, ³*J*=4.8 Hz, 3H), 1.81-1.95 (m, 1H), 3.02-3.16 (m, 2H), 3.42 (dd, ²*J*=8.7 Hz, ³*J*=7.5 Hz, 1H), 3.91 (t, ³*J*=8.7 Hz, 1H), 5.48 (t, ³*J*=8.4 Hz, 1H), 7.32-7.41 (m, 5H); ¹³C NMR (75 MHz, CDCl₃) δ 19.7, 19.8, 26.7, 51.6, 52.6, 74.1, 125.3, 128.5, 128.7, 138.8, 158.0; ESI-MS calcd for C₁₃H₁₇NO₂ 219.13, found 461.22 (2M + Na)⁺, 679.70 (3M + Na)⁺.

3-Tert-butyl-5-phenyloxazolidin-2-one:

Colorless liquid; ¹H NMR (300 MHz, CDCl₃) δ 1.41 (s, 9H), 3.45 (t, ³*J*=8.4 Hz, 1H), 3.95 (t, ³*J*=8.7 Hz, 1H), 5.36 (t, ³*J*=8.1 Hz, 1H), 7.32-7.41 (m, 5H); ¹³C NMR (75 MHz, CDCl₃) δ 27.3, 50.9, 53.5, 73.4, 125.4, 128.5, 128.7, 138.9, 156.6; ESI-MS calcd for C₁₃H₁₇NO₂ 219.13, found 242.46 (M + Na)⁺, 259.30 (M + K)⁺.

3-Benzyl-5-phenyloxazolidin-2-one:

White crystals; ¹H NMR (300 MHz, CDCl₃) δ 3.28 (t, ³*J*=8.4 Hz, 1H), 3.75 (t, ³*J*=8.7 Hz, 1H), 4.45 (ABq, J_{AB} =15.0 Hz, Δv_{AB} =36.0 Hz, 2H), 5.43 (t, ³*J*=8.1 Hz, 1H), 7.27-7.35 (m, 10H); ¹³C NMR (75 MHz, CDCl₃) δ 48.1, 51.3, 74.3, 125.3, 127.8, 127.9, 128.6, 128.7, 135.5, 138.5, 157.8; ESI-MS calcd for C₁₆H₁₅NO₂ 253.11, found 276.44(M + Na)⁺, 781.66 (3M + Na)⁺.

3-Cyclohexyl-5-phenyloxazolidin-2-one:

White crystals; ¹H NMR (300 MHz, CDCl₃) δ 1.0-1.8 (m, 10H), 3.38 (t, ³*J*=8.4 Hz, 1H), 3.70-3.73 (m, 1H), 3.88 (t, ³*J*=8.7 Hz, 1H), 5.45 (t, ³*J*=8.4 Hz, 1H), 7.35-7.38 (m, 5H); ¹³C NMR (75 MHz, CDCl₃) δ 25.1, 25.2, 29.9, 30.3, 48.1, 52.4, 74.4, 125.3, 128.5, 128.7, 138.9, 157.0; ESI-MS calcd for C₁₅H₁₉NO₂ 245.14, found 246.27 (M + H)⁺, 757.70 (3M + Na)⁺.

3-Ethyl-5-(4-chlorophenyl)oxazolidin-2-one:

White solid; ¹H NMR (400 MHz, CDCl₃) δ 1.17 (t, ³*J*=7.3 Hz, 3H), 3.30-3.43 (m, 2H), 3.69-3.76 (m, 1H), 3.92 (t, ³*J*=8.7 Hz, 1H), 5.44 (t, ³*J*=8.0 Hz, 1H), 7.27-7.38 (m, 4H); ¹³C NMR (100 MHz, CDCl₃) δ 12.6, 38.9, 51.5, 73.6, 126.9, 129.1, 134.7, 137.4, 157.4; ESI-MS calcd for C₁₁H₁₂CINO₂ 225.67, found 451.64 (2M + H)⁺.

3-Ethyl-5-p-tolyloxazolidin-2-one:

White solid; ¹H NMR (400 MHz, CDCl₃) δ 1.18 (t, ³*J*=7.3 Hz, 3H), 1.62 (d, ³*J*=6.4 Hz, 1H),1.87 (d, ³*J*=3.2 Hz, 1H), 2.27 (dd, ³*J*=6.6 Hz, ²*J*=3.2 Hz, 1H), 2.31 (s, 3H), 2.36-2.48 (m, 2H), 7.09- 7.15 (m, 4H); ¹³C NMR (100 MHz, CDCl₃) δ 12.6, 21.2, 38.9, 51.6, 74.3, 125.6, 129.5, 135.8, 138.7, 157.7; ESI-MS calcd for C₁₂H₁₅NO₂ 205.25, found 206.45 (M + H)⁺, 411.15 (2M + H)⁺.

8. References :

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9. The ¹H NMR and ¹³C NMR Charts for ionic liquids

[C₄DABCO]Br: 1-butyl-4-aza-1-azaniabicyclo[2.2.2]octane bromide





 $79.02\ (100)\ [M\text{-}C_{10}H_{21}N_2]^{\text{-}}$



[C4DABCO]OH: 1-butyl-4-aza-1-azaniabicyclo[2.2.2]octane hydroxide





[C4DABCO]Cl: 1-butyl-4-aza-1-azaniabicyclo[2.2.2]octane chloride







[C₈DABCO]Br: 1-octyl-4-aza-1-azaniabicyclo[2.2.2]octane bromide





79.03 (100) [M-C₁₄H₂₉N₂]⁻



[C₈DABCO]BF₄: 1-octyl-4-aza-1-azaniabicyclo[2.2.2]octane tetrafluoroborate





ESI-MS (4.8kV): m/z (%) = 225.45 (100) $[M-BF_4]^+$







[C₈DABCO]NTf₂: 1-octyl-4-aza-1-azaniabicyclo[2.2.2]octane bis(trifluoromethylsulfonyl)imide





$280.10\ (100)\ [M\text{-}C_{14}H_{29}N_2]^{\text{-}}$



[C₈DABCO]PF₆: 1-octyl-4-aza-1-azaniabicyclo[2.2.2]octane hexafluorophosphate







145.20 (100) [M-C₁₄H₂₉N₂]⁻



[C12DABCO]Br: 1-dodecyl-4-aza-1-azaniabicyclo[2.2.2]octane bromide







79.03 (100) [M-C₈H₁₅N₂]⁻



[C₄MIm]BF₄: 1-Butyl-3-methylimidazolium tetrafluoroborate





ESI-MS (4.8 kV): m/z (%) = 139.32 (100) $[M-BF_4]^+$







[C₈MIm]Br: 1-Butyl-3-methylimidazolium bromide



ESI-MS (4.8 kV): m/z (%) = 195.46 (100) [M-Br]⁺







[C₈MIm]BF₄: 1-Octyl-3-methylimidazolium tetrafluoroborate





$87.10\ (100)\ [M\text{-}C_{12}H_{23}N_2]^{\text{-}}$



10. The ¹H NMR charts for aziridines















11. The ¹H NMR and ¹³C NMR Charts for oxazolidinones





























12. The ¹H NMR charts of dimer of 1a

