

Straightforward one-pot synthesis of benzofuroxans from *o*-halonitrobenzenes in ionic liquids

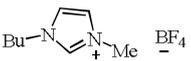
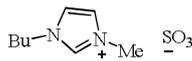
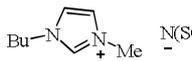
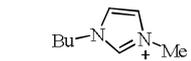
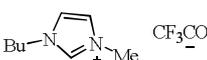
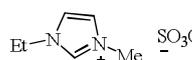
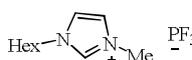
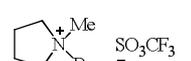
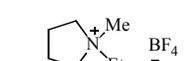
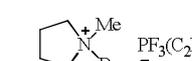
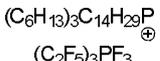
Aleksei B. Sheremetev,^{*} Nataliya S. Aleksandrova, Nikolai V. Ignat'ev and Michael Schulte

Table S1 Reactions conditions for azidation/cyclization of compound **1a**.

| NN | Comp. 1 (mmol) | NaN ₃ (mmol) | IL ^a | T, °C | Time, h | Yield, % | | | |
|----|--------------------------|----------------------------|--|-------|-----------------|----------|----------|-----------|----------|
| | | | | | | 1 | 2 | 3 | 4 |
| 1 | 0.5 | 0.51 | [bmim][BF ₄] | 20 | 72 ^b | 58 | 13 | 16 | 0 |
| 2 | 0.5 | 0.51 | [bmim][Ms] | 20 | 72 | 52 | 18 | 11 | 0 |
| 3 | 0.5 | 0.51 | [bmim][NTf ₂] | 20 | 72 | 49 | 21 | 19 | 0 |
| 4 | 0.5 | 0.51 | [bmim][Tf] | 20 | 72 | 68 | 14 | 10 | 0 |
| 5 | 1 | 1 | [bmim][CF ₃ CO ₂] | 20 | 72 | 12 | 52 | 18 | 0 |
| 6 | 1 | 1 | [bmpyrr][Tf] | 40 | 9 | 15 | 31 | 49 | 0 |
| 7 | 1 | 1 | [bmpyrr][Tf] | 60 | 3.5 | 10 | 8 | 57 | 5 |
| 8 | 1 | 1 | [bmpyrr][Tf] | 70-80 | 1.5 | 20 | 0 | 46 | 5 |
| 9 | 1 | 1.5 | [bmpyrr][Tf] | 70-80 | 1.5 | 14 | 0 | 46 | 21 |
| 10 | 1 | 2.5 | [bmpyrr][Tf] | 70-80 | 1.5 | 0 | 0 | 22 | 61 |
| 11 | 1.1 | 3.8 | [bmpyrr][Tf] | 70-80 | 2.5 | 0 | 0 | 2 | 85 |
| 12 | 1 | 1 | [empyrr][BF ₄] | 60 | 4 | trace | 0 | 95 | 0 |
| 13 | 1 | 1 | [bmpyrr][PF ₃ (C ₂ F ₅) ₃] | 60 | 10 | 97 | 0 | 0 | 0 |
| 14 | 1 | 1 | [hmim][PF ₃ (C ₂ F ₅) ₃] | 60 | 15.5 | 88 | 0 | 4 | trace |
| 15 | 1 | 1 | [bmim][NTf ₂] | 60 | 5.5 | trace | 0 | 93 | 0 |
| 16 | 1 | 1 | FAP1 | 60 | 7.5 | 91 | 0 | trace | 0 |
| 17 | 1 | 1 | [bmim][Tf] | 60 | 2 | trace | 0 | 84 | 0 |
| 18 | 1 | 1 | [emim][HSO ₄] | 60 | 10 | 95 | 0 | 0 | 0 |
| 19 | 1 | 1 | [bmim][Ms] | 60 | 4 | trace | 0 | 95 | 0 |
| 20 | 1 | 1 | [bmim][BF ₄] | 60 | 8 | trace | 0 | 65 | 0 |

^a Reaction conditions: 1 mmol of compound **1** in 2 ml of IL indicated. ^b It was found that the percentage conversion after stirring for 24 h at ambient temperature was approximately the same as that for stirring for 312 h at the same temperature.

Used Ionic Liquids

| | | | |
|---|---|--|---|
|  [bmim][BF ₄] |  [bmim][Ms] |  [bmim][NTf ₂] |  [bmim][Tf] |
|  [bmim][CF ₃ CO ₂] |  [emim][HSO ₄] |  [hmim][PF ₃ (C ₂ F ₅) ₃] | |
|  [bmpyrr][Tf] |  [empyrr][BF ₄] |  [bmpyrr][PF ₃ (C ₂ F ₅) ₃] |  FAP1 |