

Supplementary Materials

Thermal and Electrochemical Properties of Ionic Liquids Bearing Allyl Group with Sulfonate-Based Anions—Application Potential in Epoxy Resin Curing Process

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This document includes the synthetic procedure for compounds **1-4** from the manuscript. According to the synthetic procedure in the paper previously published by us [1], the following compounds were obtained:

S1 - 1-Allyl-3-methylimidazolium methylsulfate (**1**)

S2 - 1-Allyl-3-methylimidazolium methanesulfonate (**2**)

S3 - 1-Allyl-3-methylimidazolium triflate (**3**)

S4 - 1-Allyl-3-methylimidazolium tosylate (**4**)

S1 - 1-Allyl-3-methylimidazolium methylsulfate (1)

Yellow liquid; yield: 99%; purity: 98.4%.

^1H NMR (400 MHz, DMSO- d_6): δ = 9.11 (s, 1H), 7.73 (dt, 3J = 7.6 Hz, 3J = 1.8 Hz, 2H), 6.05 (ddt, 3J = 16.3 Hz, 3J = 10.3 Hz, 3J = 6.0 Hz, 1H), 5.32 (ddd, 3J = 6.7 Hz, 3J = 4.1 Hz, 3J = 1.3 Hz, 2H), 4.85 (d, 3J = 6.0 Hz, 2H), 3.88 (s, 3J = 7.4 Hz, 3H), 3.41 (s, 3H).

$^{13}\text{C} \{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6): δ = 137.35, 132.23, 124.23, 122.77, 120.66, 53.43, 51.20, 36.13.

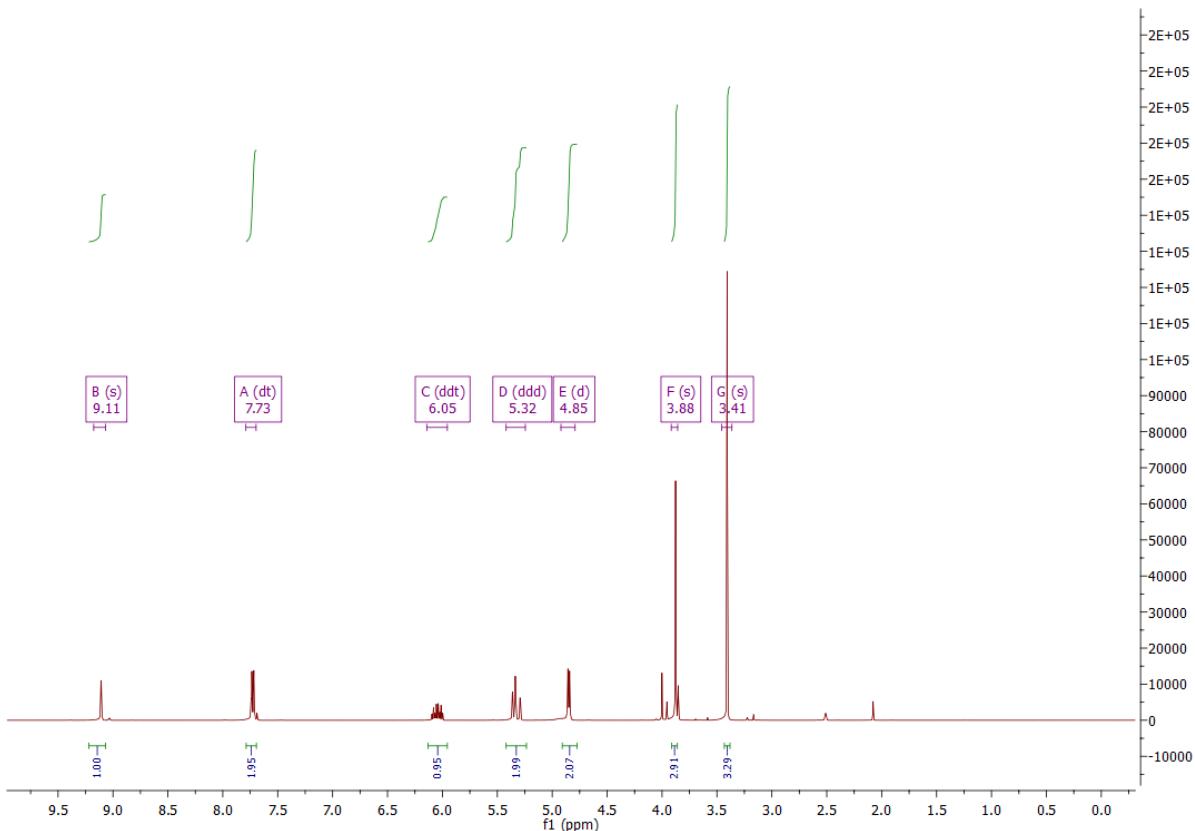


Figure S1a. ^1H NMR (400 MHz, DMSO- d_6) of 1.

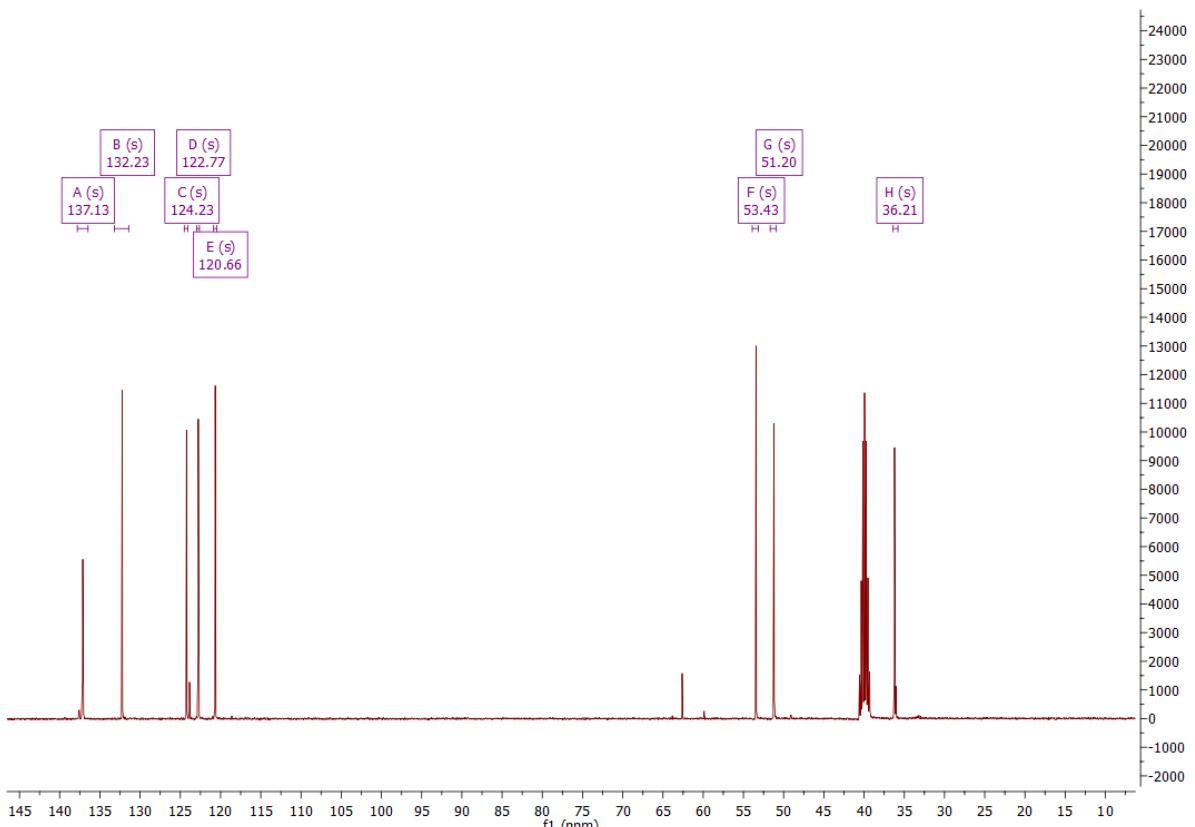


Figure S1b. $^{13}\text{C} \{^1\text{H}\}$ NMR (100 MHz, DMSO- d_6) of 1.

S2 - 1-Allyl-3-methylimidazolium methanesulfonate (2)

Yellow liquid; yield: 99.2%; purity: 99.3%.

¹H NMR (400 MHz, CDCl₃): δ = 9.63 (s, 1H), 7.52 (s, 1H), 7.37 (s, 1H), 5.90 (ddt, ³J = 16.5 Hz, ³J = 10.2 Hz, ³J = 6.3 Hz, 1H), 5.31 (t, ³J = 13.3 Hz, 2H), 4.79 (d, ³J = 6.2 Hz, 2H), 3.91 (s, 3H), 2.61 (s, 3H).

¹³C {¹H} NMR (100 MHz, CDCl₃): δ = 137.63, 130.22, 123.75, 122.02, 121.97, 51.66, 36.29.

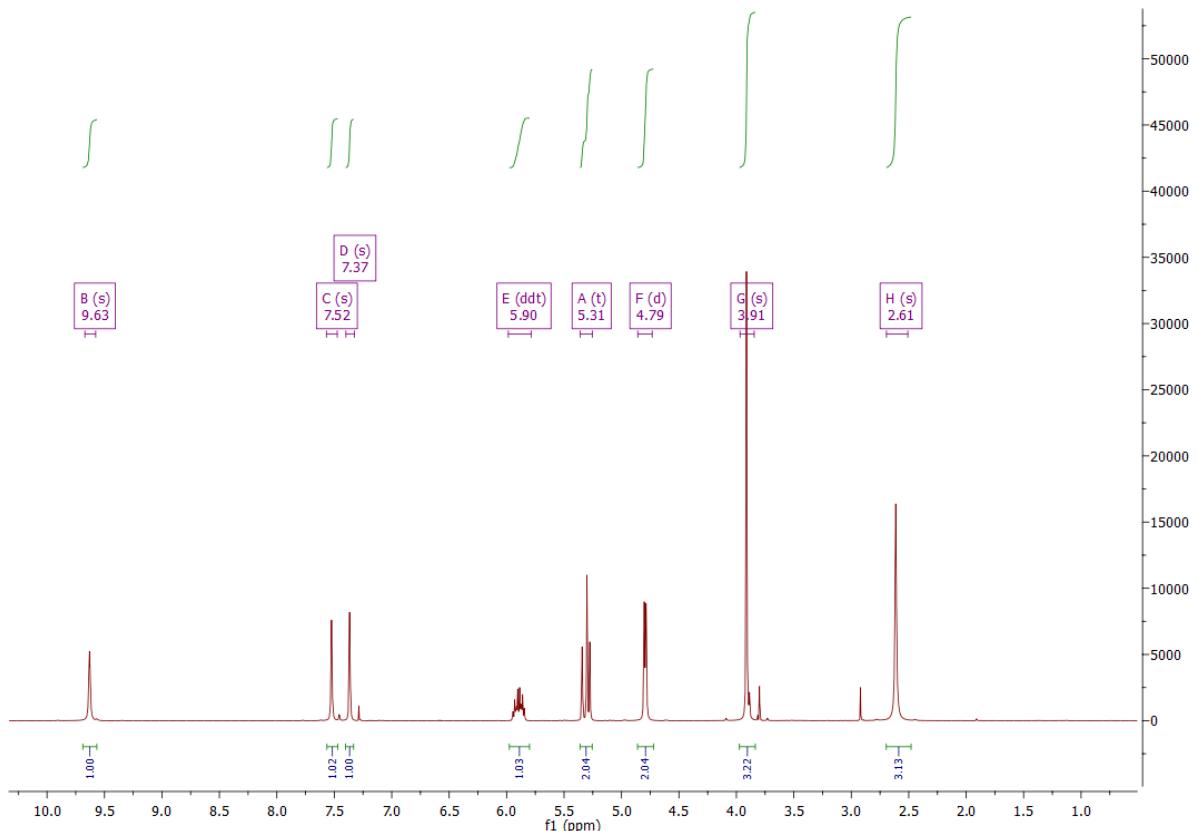


Figure S2a. ¹H NMR (400 MHz, CDCl₃) of 2.

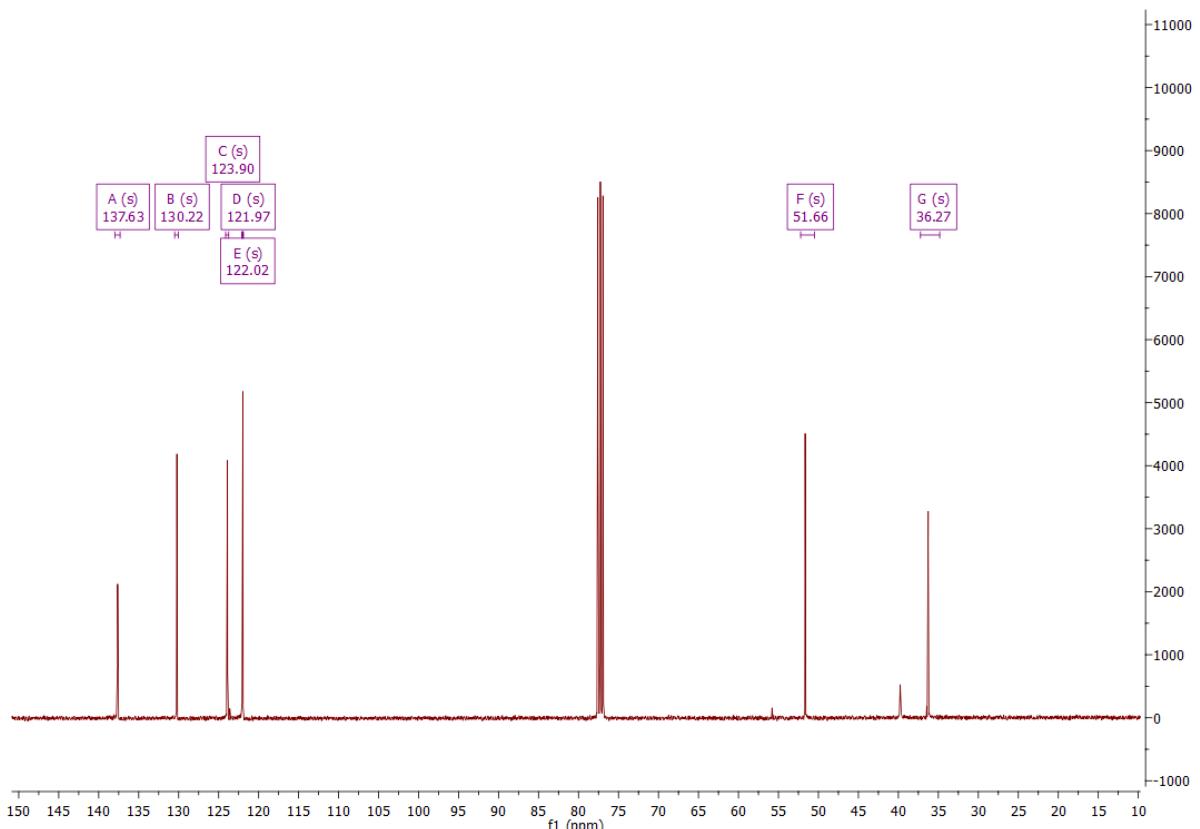


Figure S2b. ¹³C {¹H} NMR (100 MHz, CDCl₃) of 2.

S3 - 1-Allyl-3-methylimidazolium triflate (3)

Yellow liquid; yield: 99.5%; purity: 99.5%.

^1H NMR (400 MHz, DMSO- d_6): δ = 9.06 (s, 1H), 7.69 (dt, 3J = 7.2 Hz, 3J = 1.7 Hz, 2H), 6.03 (ddt, 3J = 16.3 Hz, 3J = 10.3 Hz, 3J = 6.0 Hz, 1H), 5.35 (dt, 3J = 5.0 Hz, 3J = 2.5 Hz, 1H), 5.30 (dd, 3J = 17.1 Hz, 3J = 1.3 Hz, 1H), 4.83 (d, 3J = 6.0 Hz, 2H), 3.86 (s, 3H)

^{19}F NMR (376 MHz, DMSO- d_6): δ = -77.87

^{13}C { ^1H } NMR (100 MHz, DMSO- d_6): δ = 137.04, 132.06, 124.19, 122.72, 121.10 (q, 3J = 322.1 Hz), 120.64, 51.24, 36.0.

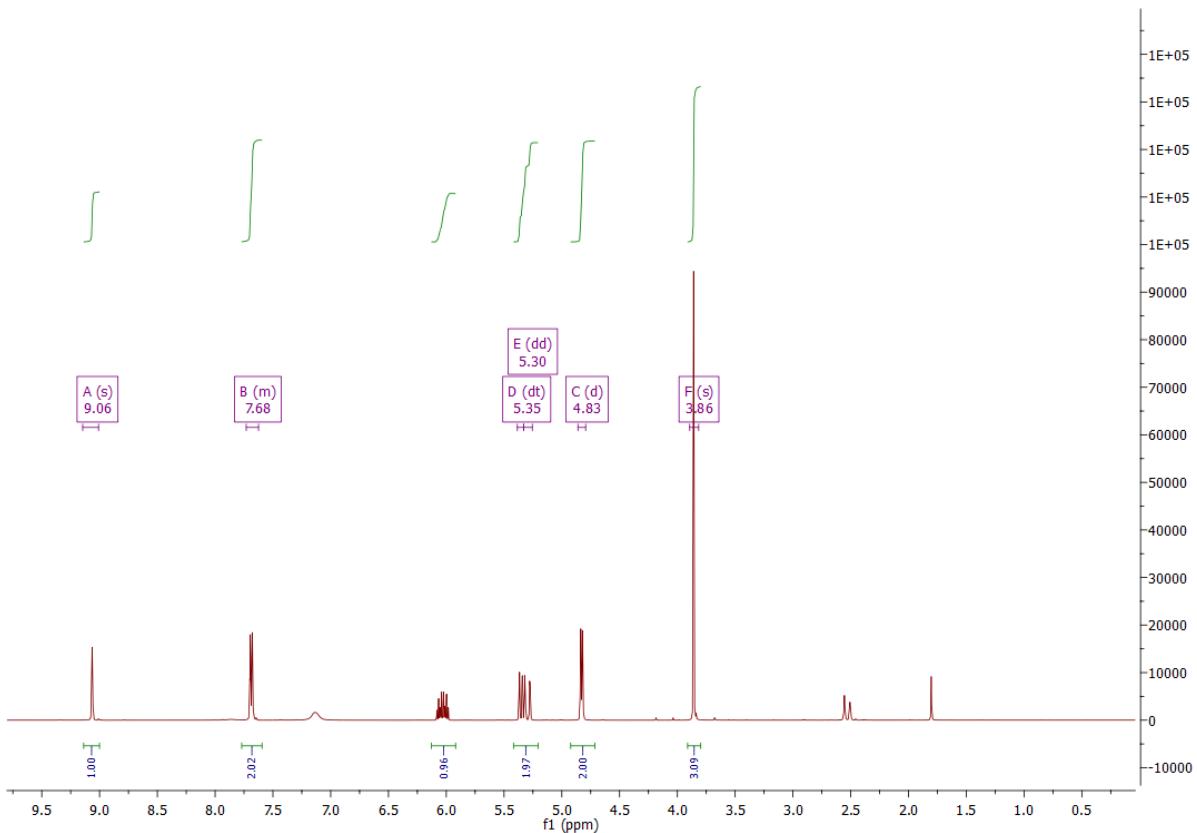


Figure S3a. ^1H NMR (400 MHz, DMSO- d_6) of 3.

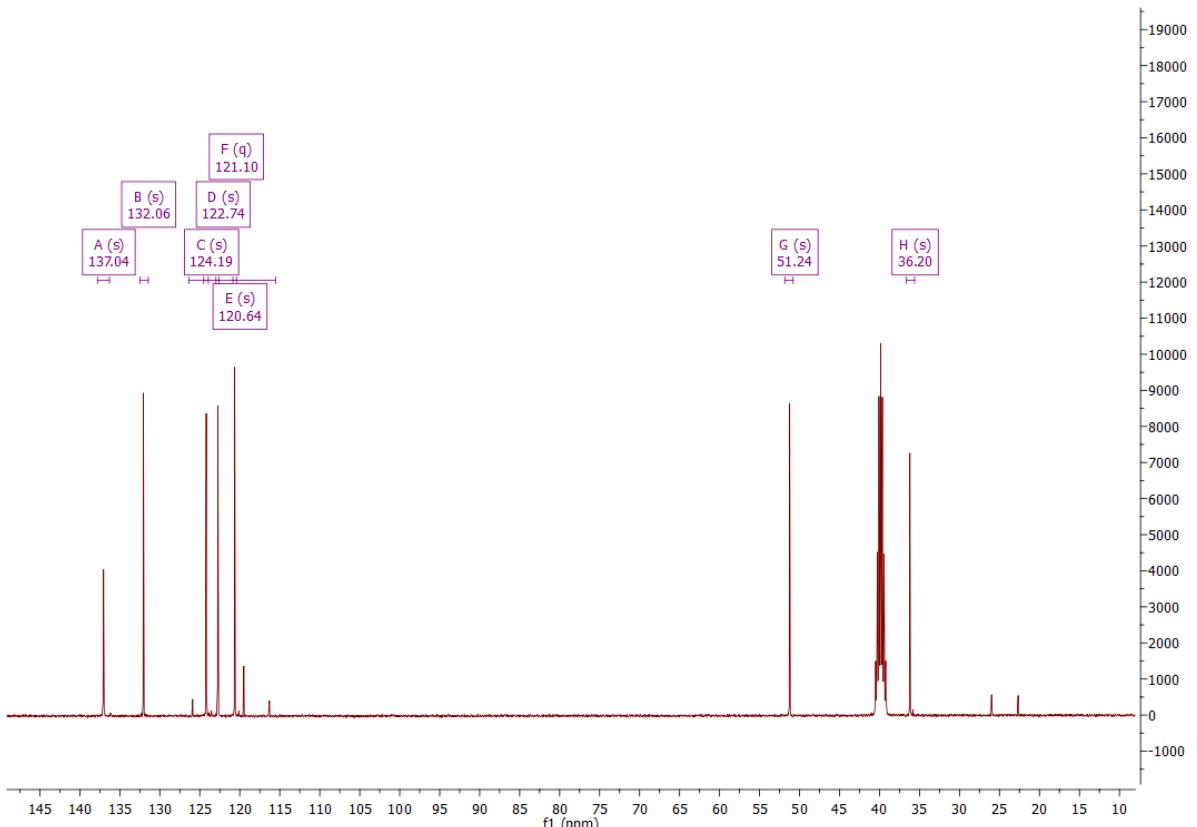


Figure S3b. ^{13}C { ^1H } NMR (100 MHz, DMSO- d_6) of 3.

S4 - 1-Allyl-3-methylimidazolium tosylate (4)

Yellow liquid; yield: 99.1%; purity: 99.2%.

^1H NMR (400 MHz, CDCl_3): δ = 9.50 (s, 1H), 7.66 (d, 3J = 7.5 Hz, 2H), 7.46 (s, 1H), 7.29 (s, 1H), 7.07 (d, 3J = 7.3 Hz, 2H), 5.82 (ddt, 3J = 16.5 Hz, 3J = 10.2 Hz, 3J = 6.3 Hz, 1H), 5.25 (dd, 3J = 13.6 Hz, 3J = 7.2 Hz, 2H), 4.69 (d, 3J = 6.2 Hz, 2H), 3.81 (s, 3H), 2.27 (s, 3H).

^{13}C { ^1H } NMR (100 MHz, CDCl_3): δ = 139.39, 137.34, 130.18, 128.66, 125.70, 123.92, 121.98, 121.90, 51.61, 36.20, 21.22.

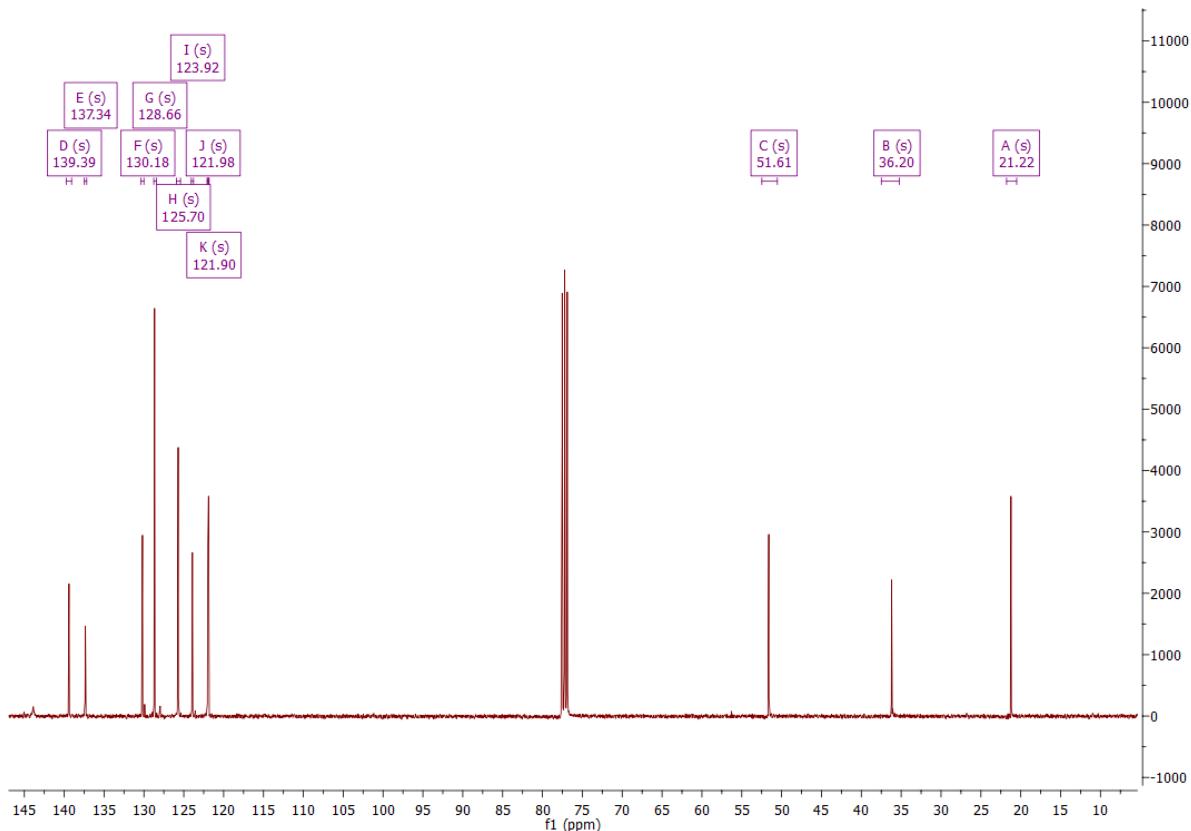


Figure S4a. ^1H NMR (400 MHz, CDCl_3) of 4.

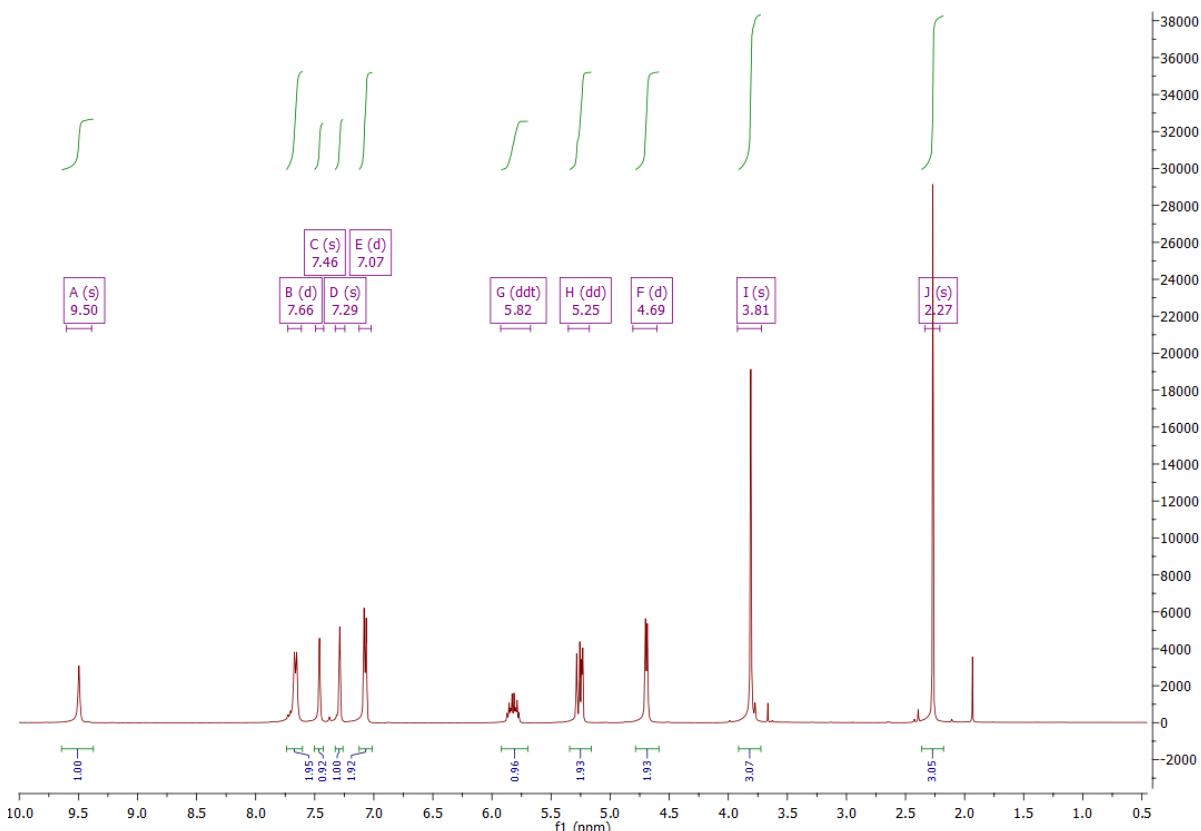


Figure S4b. ^{13}C { ^1H } NMR (100 MHz, CDCl_3) of 4.

References

1. Szpecht, A.; Zajac, A.; Zielinski, D.; Maciejewski, H.; Smiglak, M. Versatile Method for the Simultaneous Synthesis of Two Ionic Liquids, Otherwise Difficult to Obtain, with High Atom Economy. *ChemistryOpen* **2019**, *8*, 972–983, doi:10.1002/open.201900217.