SUPPLEMENTARY INFORMATION

AMMONIUM-, PHOSPHONIUM- AND SULFONIUM-BASED 2-CYANOPYRROLIDINE IONIC LIQUIDS
FOR CARBON DIOXIDE FIXATION

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Table S1. The main vibration bands of all of the investigated cations in comparison with experimental data.\textsuperscript{1,2} Abbreviations: “sm” – symmetric stretching; “as” – anti-symmetric stretching; “sc” – scissoring; “st” – stretching.

| Bond          | N0 | N2  | N3  | N4  | Experimental data |
|---------------|----|-----|-----|-----|-------------------|
| O-H           | n/a| n/a | 101 | 157 | 89 152           |
| N-O\textsubscript{sm} | n/a| 239 | 193 |     | 210               |
| C-CO\textsubscript{2} | n/a| 816 | 834 | 841 | 900-980*          |
| C-N           | 864| 828 | 855 | 753 | 800-950**         |
| C-O\textsubscript{sm} | n/a| 1322| 1334| 1333| 1337             |
| C-H\textsubscript{sc} | 1529| 1543| 1545| 1498| 1504              |
| C-O\textsubscript{as} | n/a| 1747| 1693| 1697| 1670-1720*        |

|                      | P0 | P2  | P3  | P4  |
|----------------------|----|-----|-----|-----|
| O-H                  | n/a| 54  | 54  | 26-54| Non-covalent     |
| P-O\textsubscript{sm} | n/a| 159 | 200 | 158 | Non-covalent     |
| C-CO\textsubscript{2} | n/a| 914 | 914 | 810 | 900-980*         |
| C-P                  | 1005| 995 | 632 | 480 | 900-950***       |
| C-O\textsubscript{sm} | n/a| 1333| 1333| 1305| 1318             |
| C-H\textsubscript{sc} | 1350-1428| 1353-1483| 1450-1483| 1401-1514| not used      |
|        | C-O<sub>as</sub> |     |     |     |     |
|--------|-----------------|-----|-----|-----|-----|
|        | n/a             | 1746| 1746| 1696| 1670-1720* |
|        |                 |     |     |     | C=O st    |
|        | S0              | S2  | S3  | S4  |     |
| O-H    | n/a             | 51  | 50  | 17  | Non-covalent |
|        |                 |     |     | 33  |     |
| S-O<sub>sm</sub> | n/a             | 186 | 218 | 127 | Non-covalent |
|        |                 |     |     | 172 |     |
| C-CO<sub>2</sub> | n/a             | 804 | 819 | 612 | 900-980* |
|        |                 |     |     | 623 |     |
|        |                 |     |     | 824 |     |
|        |                 |     |     | 825 |     |
| C-S    | 662-702         | no pronounced | 581-615 | 389-424 | 600**** |
| C-O<sub>sm</sub> | n/a             | 1311| 1342| 1320| 1200-1350* |
|        |                 |     |     | 1327| (C-O alkyl group) |
| C-H<sub>sc</sub> | 1426-1498       | 1362-1494 | 1360-1492 | 1343-1509 | not used |
| C-O<sub>as</sub> | n/a             | 1752| 1726| 1704| 1670-1720* |
|        |                 |     |     | 1713| C=O st    |

*Acetic acid, **Tetramethylammonium Chloride, ***Tetrabutylphosphonium bromide, ****Ethanethiol.

**REFERENCES**

(1)  *NIST Chemistry WebBook*. https://webbook.nist.gov, 2022.
(2)  *Beauchamp Spectroscopy Tables*, 2009.