

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^{1,2}. Abbreviations: “sm” – symmetric stretching; “as” – anti-symmetric stretching; “sc” – scissoring; “st” – stretching.

Bond	Frequencies, cm ⁻¹				Experimental data
	N0	N2	N3	N4	
O-H	n/a	n/a	101 157	89 152	Non-covalent
N-O _{sm}	n/a	239	193	210	Non-covalent
C-CO ₂	n/a	816	834	841 841	900-980*
C-N	864	828 971	855	753	800-950**
C-O _{sm}	n/a	1322	1334	1333 1337	1200-1350* (C-O alkyl group)
C-H _{sc}	1529	1543	1545	1498 1504	not used
C-O _{as}	n/a	1747	1693	1697 1707	1670-1720* (C=O st)
	P0	P2	P3	P4	
O-H	n/a	54	54	26-54	Non-covalent
P-O _{sm}	n/a	159	200	158	Non-covalent
C-CO ₂	n/a	914	914	810 822	900-980*
C-P	1005	995	632 992	480	900-950***
C-O _{sm}	n/a	1333	1333	1305 1318	1200-1350* (C-O alkyl group)
C-H _{sc}	1350-1428	1353-1483	1450-1483	1401-1514	not used

				1696 1707	1670-1720* C=O st
	S0	S2	S3	S4	
C-O _{as}	n/a	1746	1746		
O-H	n/a	51	50	17 33	Non-covalent
S-O _{sm}	n/a	186	218	127 172	Non-covalent
C-CO ₂	n/a	804	819	612 623 824 825	900-980*
C-S	662-702	no pronounced	581-615	389-424	600*****
C-O _{sm}	n/a	1311	1342	1320 1327	1200-1350* (C-O alkyl group)
C-H _{sc}	1426-1498	1362-1494	1360-1492	1343-1509	not used
C-O _{as}	n/a	1752	1726	1704 1713	1670-1720* 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.