

Supporting Information

Theory Study on Na⁺ Solvation in Carbonate Ester and Ether Solvents for Sodium Ion Battery

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Table S1 Length of all Na-O bonds after optimization for nEC-Na⁺ complexes, units are Å.

EC-Na ⁺	2.12 (Na-O)	-	-	-	-
2EC-Na ⁺	2.16	2.16	-	-	-
3EC-Na ⁺	2.21	2.21	2.21	-	-
4EC-Na ⁺	2.26	2.26	2.26	2.27	-
5EC-Na ⁺	2.26	2.27	2.26	2.33	5.44

Table S2 Length of C=O bonds after optimization for nEC-Na⁺ complexes, units are Å.

EC-Na ⁺	1.217 (C=O)	-	-	-	-
2EC-Na ⁺	1.211	1.211	-	-	-
3EC-Na ⁺	1.205	1.205	1.205	-	-
4EC-Na ⁺	1.201	1.201	1.2	1.201	-
5EC-Na ⁺	1.204	1.202	1.205	1.203	1.199

Table S3 Length of all Na-O bonds after optimization for nPC-Na⁺ complexes, units are Å.

PC-Na ⁺	2.11	-	-	-	-
2PC-Na ⁺	2.16	2.16	-	-	-
3PC-Na ⁺	2.21	2.21	2.21	-	-
4PC-Na ⁺	2.26	2.26	2.26	2.27	-
5PC-Na ⁺	2.26	2.29	2.26	2.32	5.02

Table S4 Length of C=O bonds after optimization for nPC-Na⁺ complexes, units are Å.

PC-Na ⁺	1.218 (C=O)	-	-	-	-
2PC-Na ⁺	1.213	1.213	-	-	-
3PC-Na ⁺	1.206	1.206	1.206	-	-
4PC-Na ⁺	1.201	1.202	1.202	1.201	-
5PC-Na ⁺	1.204	1.203	1.207	1.205	1.199

Table S5 Length of all Na-O bonds after optimization for nDEC-Na⁺ complexes, units are Å.

DEC-Na ⁺	2.11 (Na-O)	-	-	-	-
2DEC-Na ⁺	2.15	2.15	-	-	-
3DEC-Na ⁺	2.21	2.21	2.23	-	-
4DEC-Na ⁺	2.26	2.29	2.27	2.28	-
5DEC-Na ⁺	2.26	2.26	2.26	2.26	4.65

Table S6 Length of C=O bonds after optimization for nDEC-Na⁺ complexes, units are Å.

DEC-Na ⁺	1.238 (C=O)	-	-	-	-
2DEC-Na ⁺	1.233	1.233	-	-	-
3DEC-Na ⁺	1.222	1.226	1.226	-	-
4DEC-Na ⁺	1.217	1.221	1.218	1.221	-

5DEC-Na ⁺	1.221	1.221	1.22	1.216	1.211
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Table S7 Length of all Na-O bonds after optimization for nDMC-Na⁺ complexes, units are Å.

DMC-Na ⁺	2.12	-	-	-	-
2DMC-Na ⁺	2.16	2.16	-	-	-
3DMC-Na ⁺	2.21	2.21	2.21	-	-
4DMC-Na ⁺	2.27	2.27	2.27	2.28	-
5DMC-Na ⁺	2.33	2.35	2.36	2.34	2.4

Table S8 Length of C=O bonds after optimization for nDMC-Na⁺ complexes, units are Å.

DMC-Na ⁺	1.236 (C=O)	-	-	-	-
2DMC-Na ⁺	1.232	1.232	-	-	-
3DMC-Na ⁺	1.226	1.226	1.226	-	-
4DMC-Na ⁺	1.222	1.222	1.222	1.222	-
5DMC-Na ⁺	1.212	1.217	1.212	1.216	1.213

Table S9 Length of all Na-O bonds after optimization for nEMC-Na⁺ complexes, units are Å.

EMC-Na ⁺	2.12 (Na-O)	-	-	-	-
2EMC-Na ⁺	2.15	2.15	-	-	-
3EMC-Na ⁺	2.21	2.21	2.21	-	-
4EMC-Na ⁺	2.27	2.27	2.27	2.27	-
5EMC-Na ⁺	2.26	2.29	2.29	2.26	4.59

Table S10 Length of C=O bonds after optimization for all nEMC-Na⁺ complexes, units are Å.

EMC-Na ⁺	1.237 (C=O)	-	-	-	-
2EMC-Na ⁺	1.232	1.232	-	-	-
3EMC-Na ⁺	1.227	1.227	1.227	-	-
4EMC-Na ⁺	1.222	1.222	1.222	1.222	-

5EMC-Na ⁺	1.215	1.215	1.221	1.218	1.21
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Table S11 Length of all Na-O bonds after optimization for nDOL-Na⁺ complexes, units are Å.

DOL-Na ⁺	2.2 (Na-O)	-	-	-	-
2DOL-Na ⁺	2.23	2.23	-	-	-
3DOL-Na ⁺	2.27	2.27	2.27	-	-
4DOL-Na ⁺	2.33	2.29	2.32	2.32	-
5DOL-Na ⁺	2.38	2.43	2.39	2.42	2.39

Table S12 Length of C-O bonds in C-O-C group closing to O-Na bond after optimization for nDOL-Na⁺ complexes, units are Å.

DOL-Na ⁺	1.471 (C-O)	-	-	-	-
2DOL-Na ⁺	1.464	1.464	-	-	-
3DOL-Na ⁺	1.456	1.453	1.456	-	-
4DOL-Na ⁺	1.448	1.435	1.44	1.441	-
5DOL-Na ⁺	1.43	1.439	1.436	1.451	1.442

Table S13 Length of all Na-O bonds after optimization for nTHF-Na⁺ complexes, units are Å.

THF-Na ⁺	2.18 (Na-O)	-	-	-	-
2THF-Na ⁺	2.21	2.21	-	-	-
3THF-Na ⁺	2.26	2.26	2.26	-	-
4THF-Na ⁺	2.31	2.31	2.31	2.31	-
5THF-Na ⁺	2.39	2.4	2.39	2.4	2.35

Table S14 Length of all C-O bonds after optimization for nTHF-Na⁺ complexes, units are Å.

THF-Na ⁺	1.470, (C-O) 1.470 (C-O)	-	-	-	-
2THF-Na ⁺	1.465, 1.465	1.465, 1.465	-	-	-

3THF-Na ⁺	1.459, 1.460	1.459, 1.459	1.459, 1.459	-	-
4THF-Na ⁺	1.454, 1.455	1.455, 1.454	1.456, 1.453	1.456, 1.454	-
5THF-Na ⁺	1.449, 1.449	1.450, 1.450	1.451, 1.451	1.450, 1.449	1.450, 1.449

Table S15 Length of all Na-O bonds after optimization for nDME-Na⁺ complexes, units are Å.

DME-Na ⁺	2.2 (Na-O)	-	-	-	-
2DME-Na ⁺	2.23	2.23	-	-	-
3DME-Na ⁺	2.28	2.28	2.28	-	-
4DME-Na ⁺	2.34	2.35	2.35	2.34	-
5DME-Na ⁺	2.33	2.34	2.36	2.33	5.58

Table S16 Length of all C-O bonds of CH₃-O and CH₂-O closing to O-Na bond after optimization for nDME-Na⁺ complexes, units are Å.

DME-Na ⁺	1.442, (CH ₃ -O) 1.444 (CH ₂ -O)	-	-	-	-
2DME-Na ⁺	1.439, 1.441	1.439, 1.441	-	-	-
3DME-Na ⁺	1.435, 1.439	1.435, 1.439	1.435, 1.439	-	-
4DME-Na ⁺	1.432, 1.437	1.433, 1.437	1.432, 1.437	1.433, 1.437	-
5DME-Na ⁺	1.432, 1.437	1.433, 1.436	1.432, 1.438	1.432, 1.435	1.420, 1.423

Appendix 1: IR spectra vibration peaks ascription of Na⁺ solvation complexes in carbonate ester and ether solvents.

EC-Na ⁺	1801.98 cm ⁻¹ (C=O stretching)	1441.58 cm ⁻¹ , 1219.8 cm ⁻¹ (Carbonate C-O stretching and C-H twsiting)	1107.55 cm ⁻¹ (EC ring stretching)	265.51 cm ⁻¹ (O-Na stretching)		
2EC-Na ⁺	1810.7 cm ⁻¹ (C=O stretching)	1433.89 cm ⁻¹ , 1208.28 cm ⁻¹ (Carbonate C-O stretching and C-H twsiting)	1103.36 cm ⁻¹ (EC ring stretching)	315.83 cm ⁻¹ (O-Na stretching)		
3EC-Na ⁺	1830.57 cm ⁻¹ (C=O stretching)	1425.31 cm ⁻¹ , 1191.72 cm ⁻¹ (Carbonate C-O stretching and C-H twsiting)	1098.56 cm ⁻¹ (EC ring stretching)	251.03 cm ⁻¹ (O-Na stretching)		
4EC-Na ⁺	1847.93 cm ⁻¹ (C=O stretching)	1418.4 cm ⁻¹ , 1173.45 cm ⁻¹ (Carbonate C-O stretching and C-H twsiting)	1095.23 cm ⁻¹ (EC ring stretching)	217.86 cm ⁻¹ (O-Na stretching)		
5EC-Na ⁺	1837.78 cm ⁻¹ (C=O stretching)	1420.95 cm ⁻¹ , 1183.22 cm ⁻¹ (Carbonate C-O stretching and C-H twsiting)	1096.3 cm ⁻¹ (EC ring stretching)	239.45 cm ⁻¹ (O-Na stretching)		
PC-Na ⁺	1794.68 cm ⁻¹ (C=O stretching)	1440.18 cm ⁻¹ , 1239.03 cm ⁻¹ (Carbonate C-O stretching and C-H twsiting)	1100.61 cm ⁻¹ (PC ring stretching)	262.84 cm ⁻¹ (O-Na stretching)		
2PC-Na ⁺	1803.99 cm ⁻¹ (C=O stretching)	1433.34 cm ⁻¹ , 1230.26 cm ⁻¹ (Carbonate C-O stretching and C-H twsiting)	1095.05 cm ⁻¹ (PC ring stretching)	322.36 cm ⁻¹ (O-Na stretching)		
3PC-Na ⁺	1825 cm ⁻¹ (C=O stretching)	1424.82 cm ⁻¹ , 1216.69 cm ⁻¹ (Carbonate C-O stretching and C-H twsiting)	1091.9 cm ⁻¹ (PC ring stretching)	247.76 cm ⁻¹ (O-Na stretching)		
4PC-Na ⁺	1841.41 cm ⁻¹ (C=O stretching)	1422.2 cm ⁻¹ , 1204.82 cm ⁻¹ (Carbonate C-O stretching and C-H twsiting)	1092.73 cm ⁻¹ (PC ring stretching)	214.15 cm ⁻¹ (O-Na stretching)		

5PC-Na ⁺	1834.54 cm ⁻¹ (C=O stretching)	1429.49 cm ⁻¹ , 1210.21 cm ⁻¹ (Carbonate C-O stretching and C-H twsiting)	1092.2 cm ⁻¹ (PC ring stretching)	219.45 cm ⁻¹ (O-Na stretching)		
DEC-Na ⁺	1685.79 cm ⁻¹ (C=O stretching)	1521.41 cm ⁻¹ , 1458.84 cm ⁻¹ , 1421.06 cm ⁻¹ , 1340 cm ⁻¹ (C-O stretching and C-H twsiting)	1013.93 cm ⁻¹ (C-C-O stretching)	800.84 cm ⁻¹ (C-H stretching)	850.86 cm ⁻¹ (CH ₃ C-O stretching)	
2DEC-Na ⁺	1693.08 cm ⁻¹ (C=O stretching)	1516.27 cm ⁻¹ , 1454.87 cm ⁻¹ , 1421.47 cm ⁻¹ , 1336.65 cm ⁻¹ (C-O stretching and C-H twsiting)	1018.11 cm ⁻¹ (C-C-O stretching)	799.96 cm ⁻¹ (C-H stretching)	854.75 cm ⁻¹ (CH ₃ C-O stretching)	
3DEC-Na ⁺	1714.73 cm ⁻¹ (C=O stretching)	1517.45 cm ⁻¹ , 1449.31 cm ⁻¹ , 1418.68 cm ⁻¹ , 1330.4 cm ⁻¹ (C-O stretching and C-H twsiting)	1023.62 cm ⁻¹ (C-C-O stretching)	798.00 cm ⁻¹ (C-H stretching)	859.33 cm ⁻¹ (CH ₃ C-O stretching)	
4DEC-Na ⁺	1731.19-1774.24 cm ⁻¹ (C=O stretching)	1518.99 cm ⁻¹ , 1445.53 cm ⁻¹ , 1416.02 cm ⁻¹ , 1320.38 cm ⁻¹ (C-O stretching and C-H twsiting)	1025.83-1035.98 cm ⁻¹ (C-C-O stretching)	800 cm ⁻¹ (C-H stretching)	860.57 cm ⁻¹ (CH ₃ C-O stretching)	
5DEC-Na ⁺	1731.94-1778 cm ⁻¹ (C=O stretching)	1519.24 cm ⁻¹ , 1446.99 cm ⁻¹ , 1415.44 cm ⁻¹ , 1322.65 cm ⁻¹ (C-O stretching and C-H twsiting)	1024.4 cm ⁻¹ (C-C-O stretching)	797.77 cm ⁻¹ (C-H stretching)	860.64 cm ⁻¹ (CH ₃ C-O stretching)	
DMC-Na ⁺	1700.13 cm ⁻¹ (C=O stretching)	1381.79 cm ⁻¹ , 1511.64 cm ⁻¹ (C-O stretching and C-H twsiting)	967.12 cm ⁻¹ (methyl C-O stretching)	804.81 cm ⁻¹ (carbonate twisting)	302.92 cm ⁻¹ (O-Na)	
2DMC-Na ⁺	1705.17 cm ⁻¹ (C=O stretching)	1373.44 cm ⁻¹ , 1507.39 cm ⁻¹ (C-O stretching and C-H twsiting)	971.10 cm ⁻¹ (methyl C-O stretching)	803.93 cm ⁻¹ (carbonate twisting)	337.33 cm ⁻¹ (O-Na)	
3DMC-Na ⁺	1720.64 cm ⁻¹ (C=O stretching)	1363.23 cm ⁻¹ , 1503.57 cm ⁻¹ (C-O stretching and C-H twsiting)	976.16 cm ⁻¹ (methyl C-O stretching)	802.35 cm ⁻¹ (carbonate twisting)	279.72 cm ⁻¹ (O-Na)	
4DMC-Na ⁺	1732.65 cm ⁻¹ (C=O stretching)	1348.95 cm ⁻¹ , 1500.27 cm ⁻¹ (C-O stretching and C-H twsiting)	980.04 cm ⁻¹ (methyl C-O stretching)	801.96 cm ⁻¹ (carbonate twisting)	258.30 cm ⁻¹ (O-Na)	
5DMC-Na ⁺	1750.4-1806.53 cm ⁻¹ (C=O stretching)	1306.89 cm ⁻¹ , 1336.75 cm ⁻¹ , 1501.26 cm ⁻¹ (C-O stretching and C-H twsiting)	981.43 cm ⁻¹ (methyl C-O stretching)	801.85 cm ⁻¹ (carbonate twisting)	188.53 cm ⁻¹ (O-Na)	

EMC-Na ⁺	1693.03 cm ⁻¹ (C=O stretching)	1487.75 cm ⁻¹ , 1415.7 cm ⁻¹ , 1355.2 cm ⁻¹ (Carbonate C-O stretching and C-H twsiting)	1012.28 cm ⁻¹ (CH ₃ -C-O stretching)	963.97 cm ⁻¹ (CO ₃ -CH ₃ stretching)	883.12 cm ⁻¹ (CH ₃ CH ₂ -O and CH ₃ -O stretching)	802.73 cm ⁻¹ (carbonate twisting)
2EMC-Na ⁺	1699.19 cm ⁻¹ (C=O stretching)	1486.78 cm ⁻¹ , 1413.36 cm ⁻¹ , 1350.88 cm ⁻¹ (Carbonate C-O stretching and C-H twsiting)	1015.3 cm ⁻¹ (CH ₃ -C-O stretching)	963.13 cm ⁻¹ (CO ₃ -CH ₃ stretching)	884.97 cm ⁻¹ (CH ₃ CH ₂ -O and CH ₃ -O stretching)	801.92 cm ⁻¹ (carbonate twisting)
3EMC-Na ⁺	1715.75 cm ⁻¹ (C=O stretching)	1485.02 cm ⁻¹ , 1410.54 cm ⁻¹ , 1344.05 cm ⁻¹ (Carbonate C-O stretching and C-H twsiting)	1018.76 cm ⁻¹ (CH ₃ -C-O stretching)	962.94 cm ⁻¹ (CO ₃ -CH ₃ stretching)	887.45 cm ⁻¹ (CH ₃ CH ₂ -O and CH ₃ -O stretching)	800.54 cm ⁻¹ (carbonate twisting)
4EMC-Na ⁺	1731.69 cm ⁻¹ (C=O stretching)	1482.49 cm ⁻¹ , 1408.14 cm ⁻¹ , 1332.17 cm ⁻¹ (Carbonate C-O stretching and C-H twsiting)	1020.8 cm ⁻¹ (CH ₃ -C-O stretching)	961.66 cm ⁻¹ (CO ₃ -CH ₃ stretching)	888.40 cm ⁻¹ (CH ₃ CH ₂ -O and CH ₃ -O stretching)	799.61 cm ⁻¹ (carbonate twisting)
5EMC-Na ⁺	1738.68-1777.87 cm ⁻¹ (C=O stretching)	1491.97 cm ⁻¹ , 1408.2 cm ⁻¹ , 1281.14-1332.25 cm ⁻¹ (Carbonate C-O stretching and C-H twsiting)	1024.64 cm ⁻¹ (CH ₃ -C-O stretching)	956.41 cm ⁻¹ (CO ₃ -CH ₃ stretching)	889.50 cm ⁻¹ (CH ₃ CH ₂ -O and CH ₃ -O stretching)	796.21 cm ⁻¹ (carbonate twisting)
DOL-Na ⁺	3003.7-3118.81 cm ⁻¹ (C-H stretching)	1178.19cm ⁻¹ , 1112.9 cm ⁻¹ (CH ₂ twisting)	1000.38 cm ⁻¹ , 970.03 cm ⁻¹ , 937.86 cm ⁻¹ (O-CH ₂ -CH ₂ -O stretching)	841.75 cm ⁻¹ (O-C-O stretching)	244.81 cm ⁻¹ (O-Na stretching)	
2DOL-Na ⁺	2999-3116.74 cm ⁻¹ (C-H stretching)	1177.22 cm ⁻¹ , 1112,08 cm ⁻¹ (CH ₂ twisting)	1003.72 cm ⁻¹ , 972.22 cm ⁻¹ , 941.84 cm ⁻¹ (O-CH ₂ -CH ₂ -O stretching)	851.65 cm ⁻¹ (O-C-O stretching)	296.88 cm ⁻¹ (O-Na stretching)	
3DOL-Na ⁺	2992.36-3117.41 cm ⁻¹ (C-H stretching)	1178.38 cm ⁻¹ , 1111.29 cm ⁻¹ (CH ₂ twisting)	1008.25 cm ⁻¹ , 974.28 cm ⁻¹ , 944.95 cm ⁻¹ (O-CH ₂ -CH ₂ -O stretching)	867.84 cm ⁻¹ (O-C-O stretching)	252.92 cm ⁻¹ (O-Na stretching)	
4DOL-Na ⁺	2991.9-3141.79 cm ⁻¹ (C-H stretching)	1176.92 cm ⁻¹ , 1099.7 cm ⁻¹ (CH ₂ twisting)	1008.03 cm ⁻¹ , 969.70 cm ⁻¹ , 939.90 cm ⁻¹ (O-CH ₂ -CH ₂ -O stretching)	882.30 cm ⁻¹ (O-C-O stretching)	216.80-246.61 cm ⁻¹ (O-Na stretching)	

			stretching)			
5DOL-Na ⁺	2977.96- 3146.59 cm ⁻¹ (C-H stretching)	1170.97 cm ⁻¹ , 1094.65 cm ⁻¹ (CH ₂ twisting)	1011.46 cm ⁻¹ , 969.22 cm ⁻¹ , 944.10 cm ⁻¹ (O- CH ₂ -CH ₂ -O stretching)	903.95 cm ⁻¹ (O-C-O stretching)	197.74- 219.16 cm ⁻¹ (O-Na stretching)	
THF-Na ⁺	3039.59- 3124.52 cm ⁻¹ (C-H stretching)	1500.32 cm ⁻¹ , 1272.65 cm ⁻¹ , 1193.94 cm ⁻¹ (CH ₂ twisting)	847.71 cm ⁻¹ , 1018.9 cm ⁻¹ (CH ₂ -CH ₂ -O stretching)	250.01 cm ⁻¹ (O- Na stretching)		
2THF-Na ⁺	3036.29- 3122.34 cm ⁻¹ (C-H stretching)	1501.77 cm ⁻¹ , 1271.51 cm ⁻¹ , 1193.51 cm ⁻¹ (CH ₂ twisting)	867.835 cm ⁻¹ , 1027.95 cm ⁻¹ (CH ₂ -CH ₂ -O stretching)	305.28 cm ⁻¹ (O- Na stretching)		
3THF-Na ⁺	3030.06- 3119.3 cm ⁻¹ (C-H stretching)	1500.57 cm ⁻¹ , 1269.99 cm ⁻¹ , 1194.94 cm ⁻¹ (CH ₂ twisting)	876.02 cm ⁻¹ , 1036.8 cm ⁻¹ (CH ₂ -CH ₂ -O stretching)	244.72-255.03 cm ⁻¹ (O-Na stretching)		
4THF-Na ⁺	3023.52- 3116.54 cm ⁻¹ (C-H stretching)	1501.32 cm ⁻¹ , 1267.82 cm ⁻¹ , 1194.28 cm ⁻¹ (CH ₂ twisting)	881.238 cm ⁻¹ , 1050.07 cm ⁻¹ (CH ₂ -CH ₂ -O stretching)	219.58-224.5 cm ⁻¹ (O-Na stretching)		
5THF-Na ⁺	3014.61- 3114.25 cm ⁻¹ (C-H stretching)	1502.14 cm ⁻¹ , 1266.1 cm ⁻¹ , 1194.35 cm ⁻¹ (CH ₂ twisting)	889.221 cm ⁻¹ , 1060.23 cm ⁻¹ (CH ₂ -CH ₂ -O stretching)	199.36-207.54 cm ⁻¹ (O-Na stretching)		
DME-Na ⁺	2819-3128.53 cm ⁻¹ (C-H stretching)	1495.56 cm ⁻¹ , 1372.29 cm ⁻¹ , 1210.38 cm ⁻¹ (CH ₂ twisting)	1160.37 cm ⁻¹ , 1103.51 cm ⁻¹ , 1052.68 cm ⁻¹ , 931.24 cm ⁻¹ (C-O stretching)			
2DME-Na ⁺	2880.82- 3143.84 cm ⁻¹ (C-H stretching)	1497.56 cm ⁻¹ , 1372.22 cm ⁻¹ , 1210.48 cm ⁻¹ (CH ₂ twisting)	1158.55 cm ⁻¹ , 1107.95 cm ⁻¹ , 1058.19 cm ⁻¹ , 933.35 cm ⁻¹ (C-O stretching)			
3DME-Na ⁺	2929.01- 3138.88 cm ⁻¹ (C-H stretching)	1499.68 cm ⁻¹ , 1371.64 cm ⁻¹ , 1211.18 cm ⁻¹ (CH ₂ twisting)	1157.36 cm ⁻¹ , 1112.66 cm ⁻¹ , 1062.75 cm ⁻¹ , 936.19 cm ⁻¹ (C-O stretching)			
4DME-Na ⁺	2939.75- 3136.52 cm ⁻¹ (C-H stretching)	1501.83 cm ⁻¹ , 1372.04 cm ⁻¹ , 1212.38 cm ⁻¹ (CH ₂ twisting)	1156.34 cm ⁻¹ , 1115.37 cm ⁻¹ , 1064.2 cm ⁻¹ , 937.28 cm ⁻¹ (C-O stretching)			
5DME-Na ⁺	2939.42- 3135.45 cm ⁻¹ (C-H stretching)	1499.86 cm ⁻¹ , 1370.65 cm ⁻¹ , 1210.85 cm ⁻¹ (CH ₂ twisting)	1156.19 cm ⁻¹ , 1115.89 cm ⁻¹ , 1062.53 cm ⁻¹ , 935.39 cm ⁻¹ (C-O stretching)			

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Appendix 2: Raman spectra vibration peaks ascription of Na⁺ solvation complexes in carbonate ester and ether solvents.

EC-Na ⁺	3092.27-3167.9 cm ⁻¹ (C-H stretching)	1801.98 cm ⁻¹ (C=O stretching)	1523.4 cm ⁻¹ , 1241.74 cm ⁻¹ (C-H twisting)	915.75 cm ⁻¹ (EC ring enlargement stretching)	
2EC-Na ⁺	3089.83-3163.72 cm ⁻¹ (C-H stretching)	1827.34 cm ⁻¹ (C=O stretching)	1523.07 cm ⁻¹ , 1240.25 cm ⁻¹ (C-H twisting)	915.47 cm ⁻¹ (EC ring enlargement stretching)	
3EC-Na ⁺	3081.08-3158.22 cm ⁻¹ (C-H stretching)	1830.57 cm ⁻¹ , 1858.09 cm ⁻¹ (C=O stretching)	1522.61 cm ⁻¹ , 1240.28 cm ⁻¹ (C-H twisting)	913.12 cm ⁻¹ (EC ring enlargement stretching)	
4EC-Na ⁺	3074.94-3153.03 cm ⁻¹ (C-H stretching)	1848.67 cm ⁻¹ , 1882.87 cm ⁻¹ (C=O stretching)	1522.67 cm ⁻¹ , 1239.79 cm ⁻¹ (C-H twisting)	909.86 cm ⁻¹ (EC ring enlargement stretching)	
5EC-Na ⁺	3071.93-3162.49 cm ⁻¹ (C-H stretching)	1837.78-1870.01 cm ⁻¹ (C=O stretching)	1522.32 cm ⁻¹ , 1245.09 cm ⁻¹ (C-H twisting)	910.59 cm ⁻¹ (EC ring enlargement stretching)	
PC-Na ⁺	3043.16-3156.65 cm ⁻¹ (C-H stretching)	1794.68 cm ⁻¹ (C=O stretching)	1485.87-1522.62 cm ⁻¹ (C-H twisting)	649.06 cm ⁻¹ (C-C(CH ₃)-O stretching)	
2PC-Na ⁺	3042.49-3152.17 cm ⁻¹ (C-H stretching)	1821.18 cm ⁻¹ (C=O stretching)	1486.32-1522.82 cm ⁻¹ (C-H twisting)	648.04 cm ⁻¹ (C-C(CH ₃)-O stretching)	
3PC-Na ⁺	3041.72-3146.82 cm ⁻¹ (C-H stretching)	1825 cm ⁻¹ , 1853.29 cm ⁻¹ (C=O stretching)	1486.45-1523.03 cm ⁻¹ (C-H twisting)	644.81 cm ⁻¹ (C-C(CH ₃)-O stretching)	
4PC-Na ⁺	3036.2-3141.36 cm ⁻¹ (C-H stretching)	1841.41 cm ⁻¹ , 1877.88 cm ⁻¹ (C=O stretching)	1485.45-1522.65 cm ⁻¹ (C-H twisting)	642.03 cm ⁻¹ (C-C(CH ₃)-O stretching)	
5PC-Na ⁺	3038.9-3148.27 cm ⁻¹ (C-H stretching)	1861.83 cm ⁻¹ (C=O stretching)	1485.35-1524.24 cm ⁻¹ (C-H twisting)	642.38 cm ⁻¹ (C-C(CH ₃)-O stretching)	
DEC-Na ⁺	3048.73-3131.89	1497.1 cm ⁻¹ , 1296.12	1171.8 cm ⁻¹ , 1136.92	919.09 cm ⁻¹ ,	

	cm ⁻¹ (C-H stretching)	cm ⁻¹ (C-H twisting)	cm ⁻¹ (CH ₃ CH ₂ -O stretching)	350.42 cm ⁻¹ (DEC stretching)	
2DEC-Na ⁺	3049.42-3130.25 cm ⁻¹ (C-H stretching)	1498.85 cm ⁻¹ , 1297 cm ⁻¹ (C-H twisting)	1167.51 cm ⁻¹ , 1137.73 cm ⁻¹ (CH ₃ CH ₂ -O stretching)	919.30 cm ⁻¹ , 347.48 cm ⁻¹ (DEC stretching)	
3DEC-Na ⁺	3044.03-3113.93 cm ⁻¹ (C-H stretching)	1499.09 cm ⁻¹ , 1300.02 cm ⁻¹ (C-H twisting)	1162.4 cm ⁻¹ , 1138.22 cm ⁻¹ (CH ₃ CH ₂ -O stretching)	918.55 cm ⁻¹ , 348.25 cm ⁻¹ (DEC stretching)	
4DEC-Na ⁺	3039.97-3112.99 cm ⁻¹ (C-H stretching)	1497.72 cm ⁻¹ , 1299.09 cm ⁻¹ (C-H twisting)	1155.66 cm ⁻¹ , 1137.34 cm ⁻¹ (CH ₃ CH ₂ -O stretching)	917.39 cm ⁻¹ , 350.21 cm ⁻¹ (DEC stretching)	
5DEC-Na ⁺	3040.23-3113.27 cm ⁻¹ (C-H stretching)	1499.2 cm ⁻¹ , 1300.11 cm ⁻¹ (C-H twisting)	1155.93 cm ⁻¹ , 1138.18 cm ⁻¹ (CH ₃ CH ₂ -O stretching)	917.60 cm ⁻¹ , 347.79 cm ⁻¹ (DEC stretching)	
DMC-Na ⁺	3056.65-3181.08 cm ⁻¹ (C-H stretching)	1493.82 cm ⁻¹ (C-H twisting)	951.06 cm ⁻¹ (carbonate stretching)	521.27 cm ⁻¹ (DMC stretching)	
2DMC-Na ⁺	3055.43-3178.87 cm ⁻¹ (C-H stretching)	1492.68 cm ⁻¹ (C-H twisting)	948.03 cm ⁻¹ (carbonate stretching)	521.31 cm ⁻¹ (DMC stretching)	
3DMC-Na ⁺	3055.99-3176.37 cm ⁻¹ (C-H stretching)	1491.53 cm ⁻¹ (C-H twisting)	945.65 cm ⁻¹ (carbonate stretching)	517.41 cm ⁻¹ (DMC stretching)	
4DMC-Na ⁺	3053.79-3174.53 cm ⁻¹ (C-H stretching)	1492.04 cm ⁻¹ (C-H twisting)	942.69 cm ⁻¹ (carbonate stretching)	516.06 cm ⁻¹ (DMC stretching)	
5DMC-Na ⁺	3055.3-3176.93 cm ⁻¹ (C-H stretching)	1491.56 cm ⁻¹ (C-H twisting)	938.57 cm ⁻¹ (carbonate stretching)	515.59 cm ⁻¹ (DMC stretching)	
EMC-Na ⁺	3048.58-3179.27 cm ⁻¹ (C-H stretching)	1496.27 cm ⁻¹ , 1299.14 cm ⁻¹ (C-H twisting)	963.97 cm ⁻¹ (carbonate and CH ₃ -O stretching)	517.20 cm ⁻¹ (EMC stretching)	366.14 cm ⁻¹ (EMC and O-Na stretching)
2EMC-Na ⁺	3048.36-3177.49 cm ⁻¹ (C-H stretching)	1496.64 cm ⁻¹ , 1298.94 cm ⁻¹ (C-H twisting)	963.13 cm ⁻¹ (carbonate and CH ₃ -O stretching)	517.51 cm ⁻¹ (EMC stretching)	365.87 cm ⁻¹ (EMC and O-Na stretching)
3EMC-Na ⁺	3046.98-3174.76 cm ⁻¹ (C-H stretching)	1496.24 cm ⁻¹ , 1299.03 cm ⁻¹ (C-H twisting)	963.26 cm ⁻¹ (carbonate and CH ₃ -O stretching)	513.38 cm ⁻¹ (EMC stretching)	366.58 cm ⁻¹ (EMC and O-Na stretching)
4EMC-Na ⁺	3045.69-3172.38	1495.67 cm ⁻¹ , 1298.62	962.02 cm ⁻¹	510.35 cm ⁻¹	367.14 cm ⁻¹

	cm ⁻¹ (C-H stretching)	cm ⁻¹ (C-H twisting)	(carbonate and CH ₃ -O stretching)	(EMC stretching)	(EMC and O-Na stretching)
5EMC-Na ⁺	3041.14-3169.88 cm ⁻¹ (C-H stretching)	1498.91 cm ⁻¹ , 1300.32 cm ⁻¹ (C-H twisting)	963.63 cm ⁻¹ (carbonate and CH ₃ -O stretching)	511.94 cm ⁻¹ (EMC stretching)	369.30 cm ⁻¹ (EMC and O-Na stretching)
DOL-Na ⁺	3003.7-3151.09 cm ⁻¹ (C-H stretching)	1211.87-1538.1 cm ⁻¹ (C-H twisting)	1000.38 cm ⁻¹ , 970.03 cm ⁻¹ , 937.86 cm ⁻¹ (O-CH ₂ -CH ₂ -O stretching)		
2DOL-Na ⁺	2998.91-3148.64 cm ⁻¹ (C-H stretching)	1211.6-1539.82 cm ⁻¹ (C-H twisting)	1003.72 cm ⁻¹ , 972.11 cm ⁻¹ , 941.44 cm ⁻¹ (O-CH ₂ -CH ₂ -O stretching)		
3DOL-Na ⁺	2991.07-3145.2 cm ⁻¹ (C-H stretching)	1213.56-1540.8 cm ⁻¹ (C-H twisting)	1008.25 cm ⁻¹ , 973.45 cm ⁻¹ , 944.95 cm ⁻¹ (O-CH ₂ -CH ₂ -O stretching)		
4DOL-Na ⁺	2991.9-3141.79 cm ⁻¹ (C-H stretching)	1213.09-1550.18 cm ⁻¹ (C-H twisting)	969.70 cm ⁻¹ , 939.90 cm ⁻¹ (O-CH ₂ -CH ₂ -O stretching)		
5DOL-Na ⁺	2971.69-3150.86 cm ⁻¹ (C-H stretching)	1240.47-1546.82 cm ⁻¹ (C-H twisting)	971.439 cm ⁻¹ , 936.33 cm ⁻¹ (O-CH ₂ -CH ₂ -O stretching)		
THF-Na ⁺	In agreement with IR (C-H vibration)	1048.82 cm ⁻¹ , 927.1 cm ⁻¹ (C-C symmetrical vibration)	865.83 cm ⁻¹ (C-O stretching)		
2THF-Na ⁺	In agreement with IR (C-H vibration)	1048.18 cm ⁻¹ , 926.97 cm ⁻¹ (C-C symmetrical vibration)	872.92 cm ⁻¹ (C-O stretching)		
3THF-Na ⁺	In agreement with IR (C-H vibration)	1047.78 cm ⁻¹ , 927.68 cm ⁻¹ (C-C symmetrical vibration)	881.85 cm ⁻¹ (C-O stretching)		
4THF-Na ⁺	In agreement with IR (C-H vibration)	1044.48 cm ⁻¹ , 927.62 cm ⁻¹ (C-C symmetrical vibration)	889.61 cm ⁻¹ (C-O stretching)		
5THF-Na ⁺	In agreement with IR (C-H vibration)	1043.04 cm ⁻¹ , 928.28 cm ⁻¹ (C-C symmetrical vibration)	896.28 cm ⁻¹ (C-O stretching)		
DME-Na ⁺	In agreement with IR (C-H vibration)	1296.11 cm ⁻¹ (H element twisting)	In agreement with IR (C-O stretching vibration)	998.16 cm ⁻¹ (DME stretching)	399.21 cm ⁻¹ , 351.12 cm ⁻¹ (DME structure twisting)
2DME-Na ⁺	In agreement with IR	1297.45 cm ⁻¹ (H element twisting)	In agreement with IR (C-O stretching)	999.27 cm ⁻¹ (DME)	400.38 cm ⁻¹ , 340.07 cm ⁻¹

	(C-H vibration)		vibration)	stretching)	(DME structure twisting)
3DME-Na ⁺	In agreement with IR (C-H vibration)	1301.13 cm ⁻¹ (H element twisting)	In agreement with IR (C-O stretching vibration)	999.37 cm ⁻¹ (DME stretching)	399.90 cm ⁻¹ , 339.42 cm ⁻¹ (DME structure twisting)
4DME-Na ⁺	In agreement with IR (C-H vibration)	1300.5 cm ⁻¹ (H element twisting)	In agreement with IR (C-O stretching vibration)	999.28 cm ⁻¹ (DME stretching)	399.31 cm ⁻¹ , 341.79 cm ⁻¹ (DME structure twisting)
5DME-Na ⁺	In agreement with IR (C-H vibration)	1301.71 cm ⁻¹ (H element twisting)	In agreement with IR (C-O stretching vibration)	1000.81 cm ⁻¹ (DME stretching)	399.31 cm ⁻¹ , 339.61 cm ⁻¹ (DME structure twisting)