

Supporting Information

Coordination Abilities of 4,5-Dicyano-2-(trifluoromethyl)imidazolate Anion toward Sodium Cation: Structural and Spectroscopic Studies of Solid and Liquid Glyme-Solvated Electrolyte Systems

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Table S1. Crystal Data for the Single Crystal X-ray Structures of **1-8**.

Compound reference	1	2	3	4
Molecular formula	Na(12C4) ₂ ⁺ ·TDI	Na(15C5)·TDI	Na(18C6)·TDI	Na(G4)·TDI
Chemical formula	[C ₁₆ H ₃₂ NaO ₈] ⁺ [C ₆ F ₃ N ₄] ⁻	C ₁₆ H ₂₀ F ₃ N ₄ NaO ₅	C ₁₈ H ₂₄ F ₃ N ₄ NaO ₆	C ₃₂ H ₄₄ F ₆ N ₈ Na ₂ O ₁₀
Formula Mass	560.50	428.35	472.40	860.73
Crystal system	Monoclinic	Orthorhombic	Monoclinic	Triclinic
<i>a</i> /Å	18.4018(6)	9.52266(9)	9.2466(4)	15.02929(14)
<i>b</i> /Å	17.2253(4)	9.79219(10)	17.7798(8)	22.3663(2)
<i>c</i> /Å	18.0341(6)	21.7134(2)	14.7018(7)	25.7490(2)
<i>α</i> /°	90	90	90	90.0006(8)
<i>β</i> /°	113.208(4)	90	102.101(4)	90.0093(7)
<i>γ</i> /°	90	90	90	102.8619(8)
Unit cell volume/Å ³	5253.8(3)	2024.72(3)	2363.31(19)	8438.33(14)
Temperature/K	120.0(1)	100.0(3)	200.0(1)	100.0(4)
Space group	<i>C</i> 2/ <i>c</i>	<i>P</i> 2 ₁ 2 ₁	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 1̄
No. of formula units per unit cell, <i>Z</i>	8	4	4	8
Radiation type	MoKα	MoKα	MoKα	CuKα
Absorption coefficient, μ/mm ⁻¹	0.134	0.140	0.130	1.194
No. of reflections measured	31646	106149	20417	258163
No. of independent reflections	7302	4574	4190	29951
<i>R</i> _{int}	0.0343	0.0353	0.0370	0.0500
Final <i>R</i> _i values (<i>I</i> > 2σ(<i>I</i>))	0.0394	0.0220	0.0391	0.0558
Final <i>wR</i> (<i>F</i> ²) values (<i>I</i> > 2σ(<i>I</i>))	0.0846	0.0578	0.0866	0.1497
Final <i>R</i> _i values (all data)	0.0563	0.0226	0.0558	0.0593
Final <i>wR</i> (<i>F</i> ²) values (all data)	0.0932	0.0584	0.0957	0.1541
Goodness of fit on <i>F</i> ²	1.022	1.074	1.032	1.013
CCDC number	1576879	1576880	1576881	1576882

Compound reference	5	6	7	8
Molecular formula	[Na(G3)·TDI] ₂	Na(G2)·TDI	Na(G1) _{0.67} ·TDI	Na(THF)·TDI
Chemical formula	C ₂₈ H ₃₆ F ₆ N ₈ Na ₂ O ₈	C ₁₂ H ₁₄ F ₃ N ₄ NaO ₃	C ₂₆ H ₂₀ F ₉ N ₁₂ Na ₃ O ₄	C ₂₀ H ₁₆ F ₆ N ₈ Na ₂ O ₂
Formula Mass	772.63	342.26	804.51	560.39
Crystal system	Triclinic	Monoclinic	Orthorhombic	Monoclinic
<i>a</i> /Å	9.3885(2)	20.2366(3)	37.2006(3)	16.0906(2)
<i>b</i> /Å	10.2919(3)	9.67468(17)	12.80126(12)	8.89160(10)
<i>c</i> /Å	10.7572(3)	16.1201(2)	7.46127(7)	16.8789(2)
<i>α</i> /°	82.713(2)	90	90	90
<i>β</i> /°	67.371(2)	96.6933(14)	90	94.9700(10)
<i>γ</i> /°	74.624(2)	90	90	90
Unit cell volume/ Å ³	924.71(4)	3134.51(9)	3553.16(5)	2405.80(5)
Temperature/K	100.0(1)	100.0(1)	100.0(2)	100.0(2)
Space group	<i>P</i> 1̄	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> 2 ₁ 2 ₁ 2	<i>P</i> 2 ₁ / <i>n</i>
No. of formula units per unit cell, <i>Z</i>	1	8	4	4
Radiation type	MoKα	MoKα	MoKα	CuKα
Absorption coefficient, μ/mm ⁻¹	0.141	0.151	0.168	1.508
No. of reflections measured	47735	48881	169271	69456
No. of independent reflections	4400	6322	7491	4296
<i>R</i> _{int}	0.0298	0.0382	0.0533	0.0448
Final <i>R</i> _i values (<i>I</i> > 2σ(<i>I</i>))	0.0290	0.0305	0.0377	0.0313
Final <i>wR</i> (<i>F</i> ²) values (<i>I</i> > 2σ(<i>I</i>))	0.0727	0.0791	0.0983	0.0841
Final <i>R</i> _i values (all data)	0.0323	0.0374	0.0380	0.0349
Final <i>wR</i> (<i>F</i> ²) values (all data)	0.0756	0.0838	0.0986	0.0875
Goodness of fit on <i>F</i> ²	1.033	1.030	1.114	1.055
CCDC number	1576883	1576884	1576885	1576886

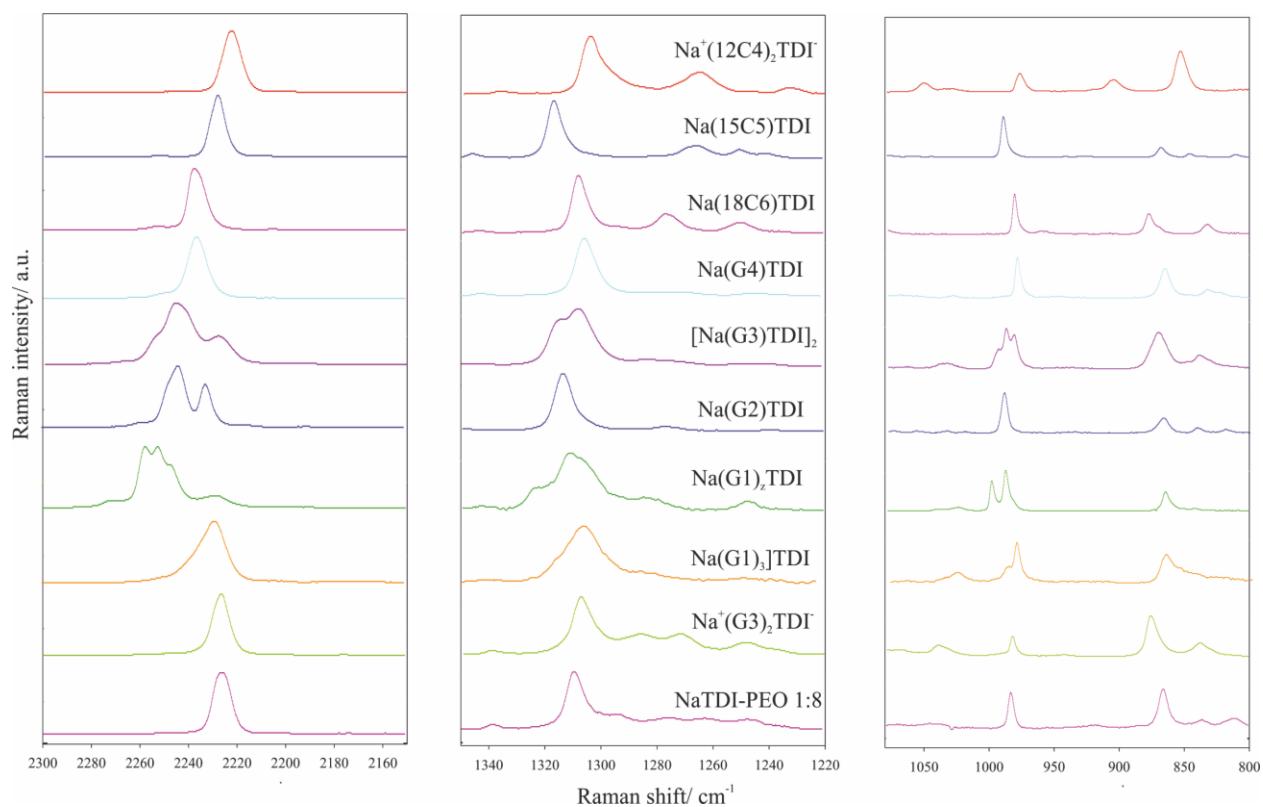


Figure S1. Raman spectra of crystalline NaTDI-glyme complexes in spectral ranges corresponding to (a) ν_{CN} , (b) $\nu_{\text{CN_Im}}$ and (c) δ_{NCN} vibrations.

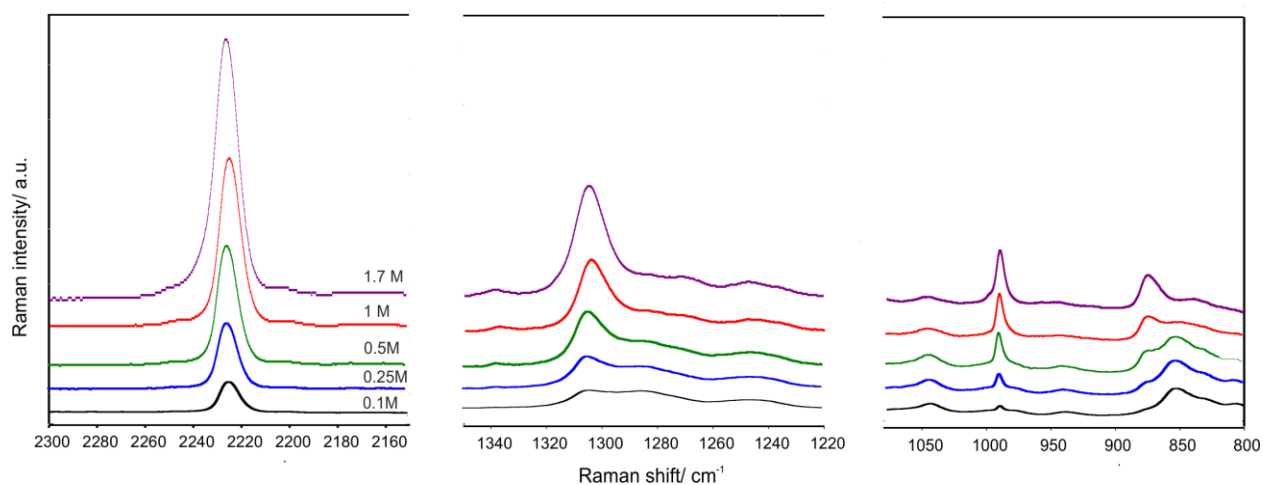


Figure S2. Raman spectra of LiTDI-G3 solutions in spectral ranges corresponding to (a) ν_{CN} , (b) $\nu_{\text{CN_Im}}$ and (c) δ_{NCN} vibrations.