Supporting Information

Urea-Enhanced Solubilization of Lithium Nitrate for Improved Lithium Metal Cycling: Experimental and Molecular Dynamics Investigation

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Table of Contents

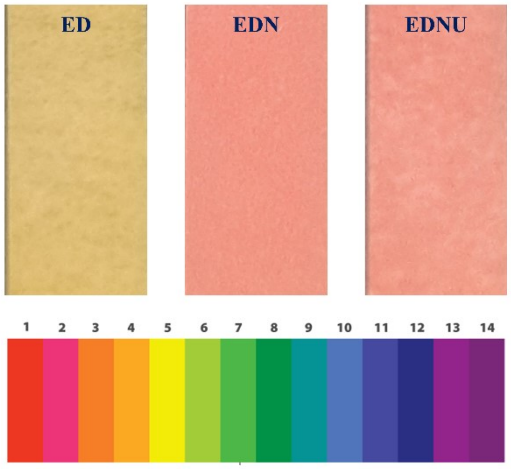

Fig. S1. pH indicator paper test results

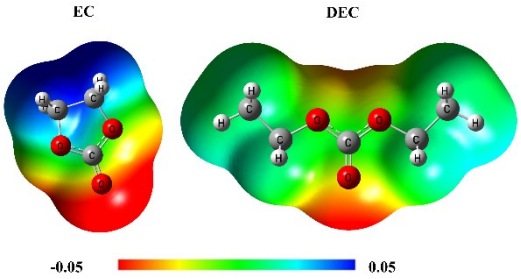

Fig. S2. Molecular electrostatic potential (ESP) maps for ethylene carbonate (EC), and diethyl carbonate (DEC) molecules.

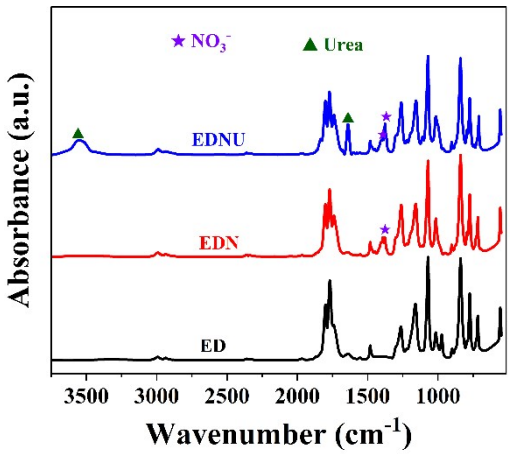

Fig. S3. FTIR analysis of electrolytes.

The FTIR spectrum confirms the molecular structure and interactions within the electrolytes. Key peaks reveal the presence and coordination of all components: the PF_6^- anion (P–F bending and asymmetric stretching modes at 557 cm^{-1} and 839 cm^{-1}), the EC carbonyl (C=O stretch at 1769 cm^{-1}), and the DEC carbonyl (C=O stretch at 1739 cm^{-1}).[1] The 1769 cm^{-1} EC peak is red-shifted from pure EC ~1780-1800 cm^{-1}), indicating significant Li^+-coordination with the EC carbonyl oxygen.[1] The introduction of $LiNO_3$ is evidenced by the NO_3^- asymmetric stretches at 1375 and 1393 cm^{-1} (in EDN and EDNU systems), which suggests significant Li^+–NO_3^- contact ion pairing. The addition of urea (EDNU) introduces distinct features: the N–H stretch at 3553 cm^{-1}, the amide II band at 1640 cm^{-1}, and the carbonyl stretch at 1667 cm^{-1}. These changes confirm that urea establishes a pervasive hydrogen-bonding network and competes

for Li^+ solvation, fundamentally reshaping the ion-pairing equilibria and solvation dynamics. Other solvent-related peaks include EC skeletal modes (710 cm^{-1}) and EC ring deformation (903 cm^{-1}).

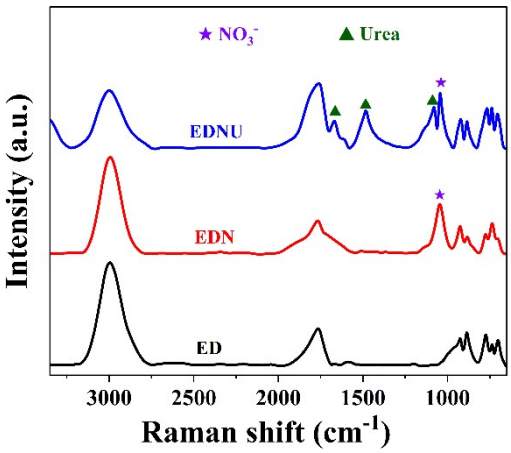

Fig. S4. Raman spectroscopy analysis of electrolytes.

The Raman spectra provide further insight into the solvation and ion-pairing behavior. In the baseline ED system, peaks at 923 cm^{-1} (for Li^+-coordinated EC) and 739/773 cm^{-1} (PF_6^- symmetric P–F stretch) characterize the initial interactions.[2] Upon $LiNO_3$ addition (EDN), a new NO_3- peak appears at 1043 cm^{-1}. The enhanced intensity of the free PF_6^- peak (shifted 739 cm^{-1}) and the diminished 773 cm^{-1} peak (contact ion pair, CIP) indicate that NO_3- effectively outcompetes PF_6^- for Li^+ coordination, thereby disrupting Li^+–PF_6^- pairing.[2,3] The subsequent addition of urea (EDNU) introduces strong peaks at 1483 and 1667cm^{-1}, confirming its involvement in N–H bending/C–N and carbonyl stretching modes. Crucially, the EC peak at 887 cm^{-1} (free EC ring breathing) becomes dominant again, and the C–H band at 2995 cm^{-1} weakens, suggesting that urea displaces EC from the Li^+ solvation shell.[3] These findings collectively demonstrate that $LiNO_3$ disrupts the initial Li^+–PF_6^- pairing, while urea further modifies the solvation landscape by coordinating with Li^+ and interacting with NO_3^-, which is vital for optimizing electrolyte performance.

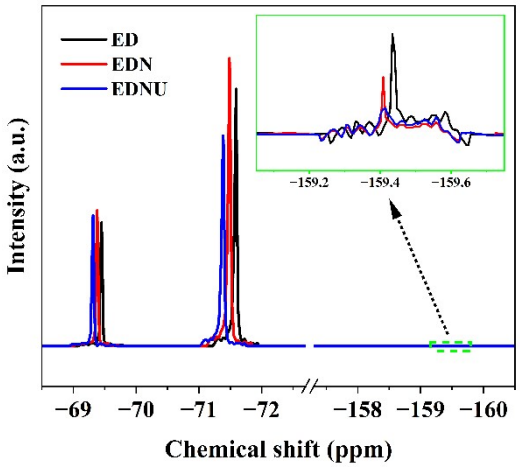

Fig. S5. ^{19}F NMR (500 MHz, DMSO-d_6 sample measurement, ref. CH_3NO_2) analysis of electrolytes

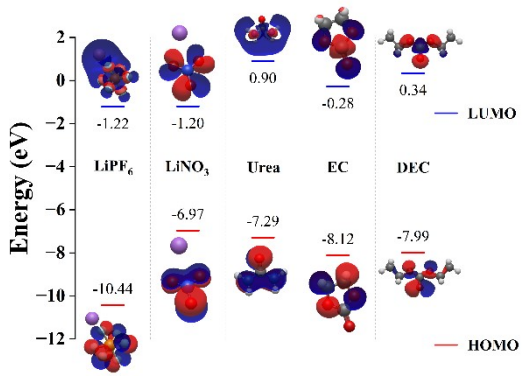

Fig. S6. Comparison of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy levels of salts and solvents studied.

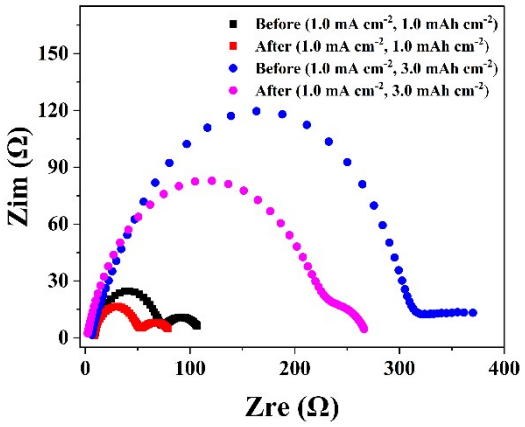

Fig. S7. Nyquist plots of Li||Li symmetric cells containing EDNU electrolyte, comparing the initial state (pre-cycling) and the final state (post-cycling) under low-depth (1 mAh cm^{-2}) and high-depth (3 mAh cm^{-2}) cycling conditions.

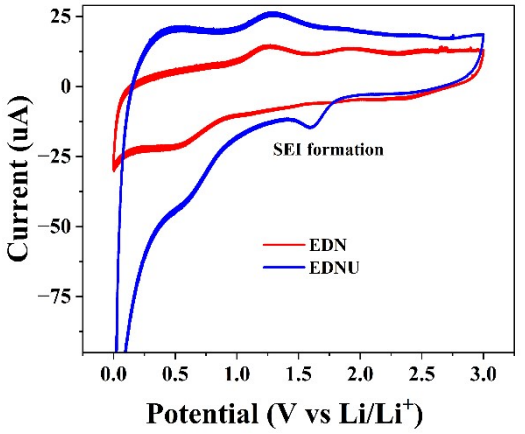

Fig. S8. Typical CV curves of Li||Cu half cells scanned between 0-3.0 V at 0.5 mV s^{-1} in EDN and EDNU electrolytes, the distinct reduction peak at 1.6 V during the cathodic scan indicates the reduction of $LiNO_3$.

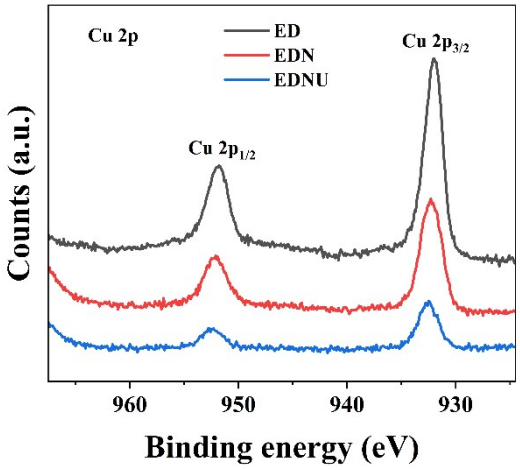

Fig. S9. High-resolution XPS spectra of Cu 2p

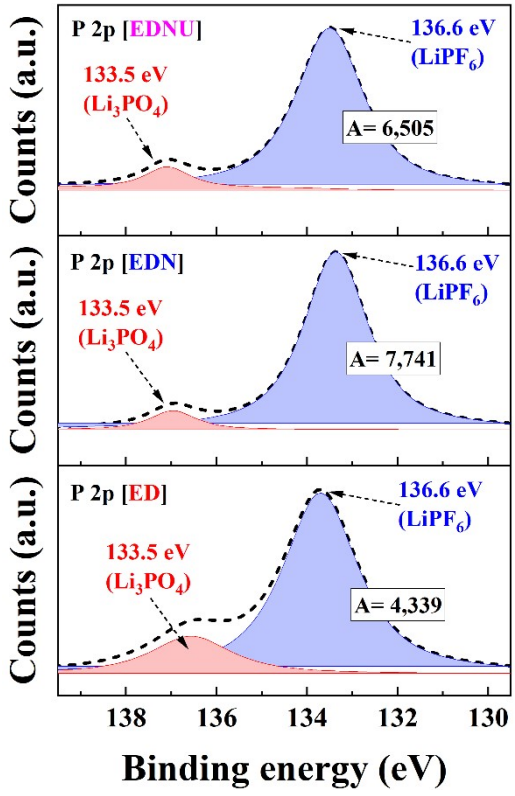

Fig. S10. High-resolution XPS spectra of P 2p

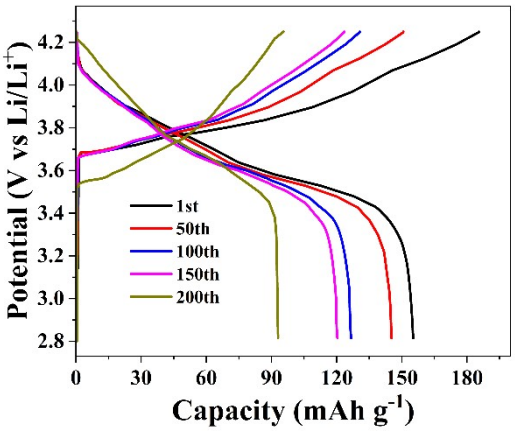

Fig. S11. Charge-discharge curves of the Li||NCM811 cell operating with the EDN electrolyte.

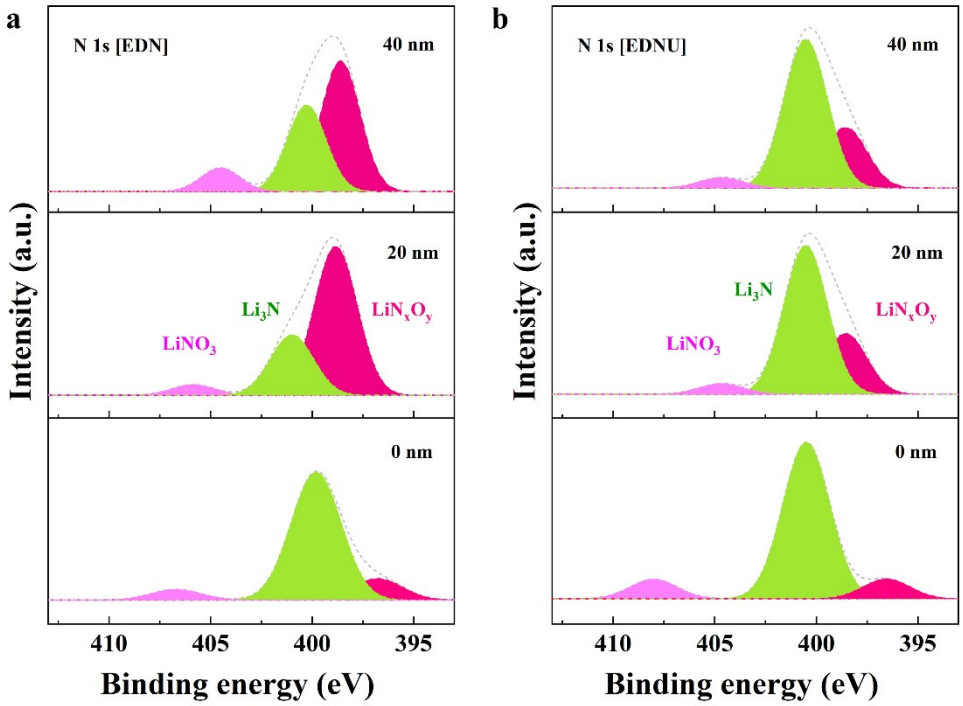

Fig. S12. The N 1s spectra of the CEI formed at different depths in (a) EDN and (b) EDNU electrolytes.

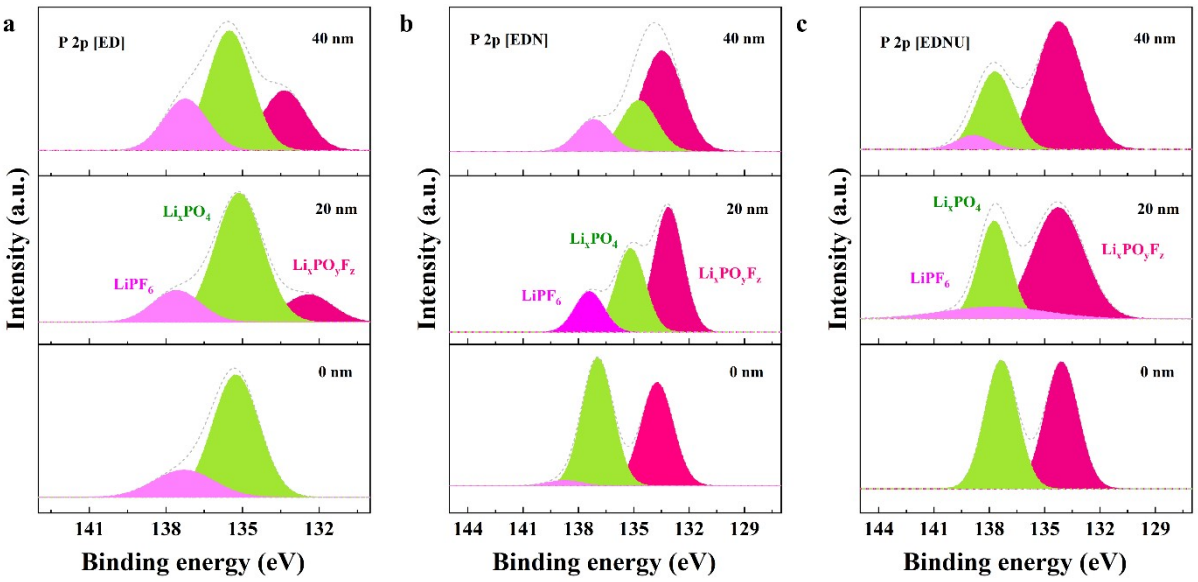

Fig. S13. The P 2p spectra of the CEI formed at different depths in (a) ED, (b) EDN and (c) EDNU electrolytes.

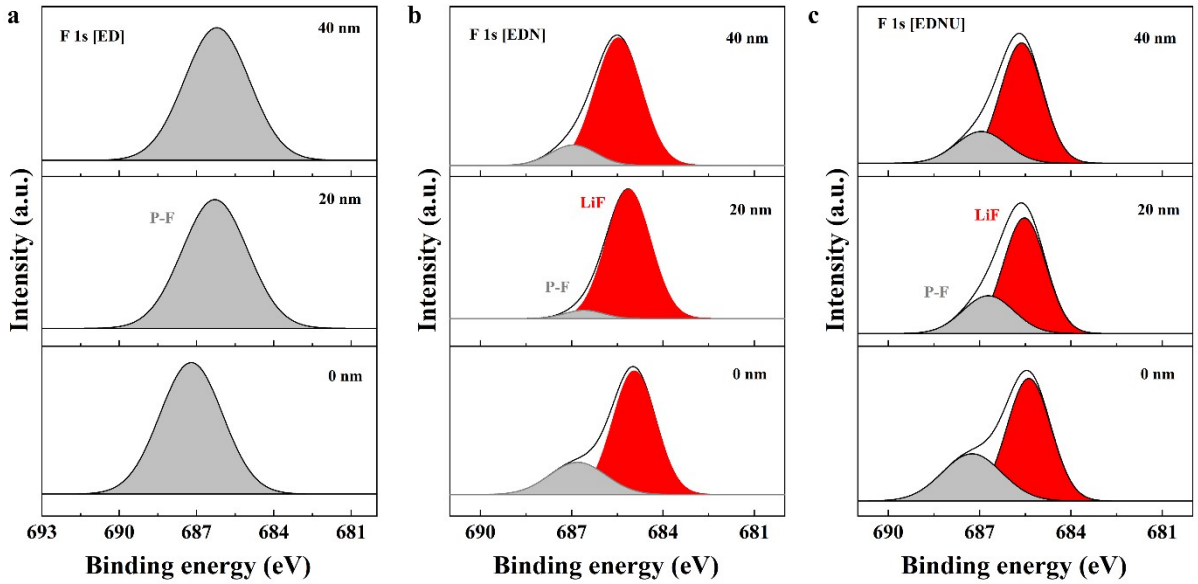

Fig. S14. The F 1s spectra of the CEI formed at different depths in (a) ED, (b) EDN and (c) EDNU electrolytes.

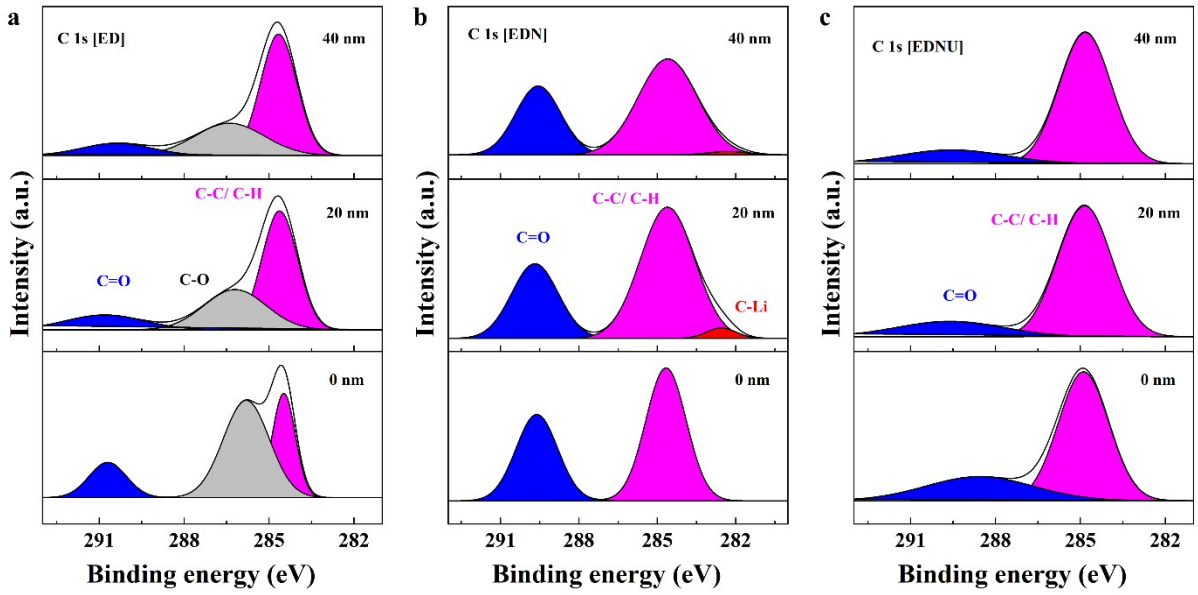

Fig. S15. The C 1s spectra of the CEI formed at different depths in (a) ED, (b) EDN and (c) EDNU electrolytes.

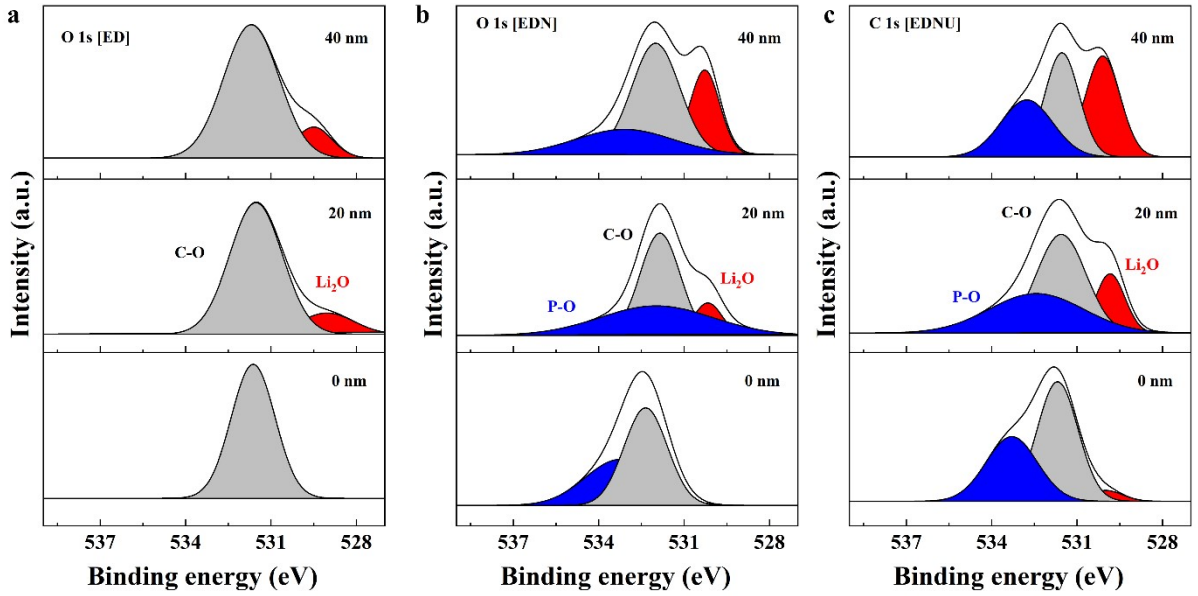

Fig. S16. The O 1s spectra of the CEI formed at different depths in (a) ED, (b) EDN and (c) EDNU electrolytes.

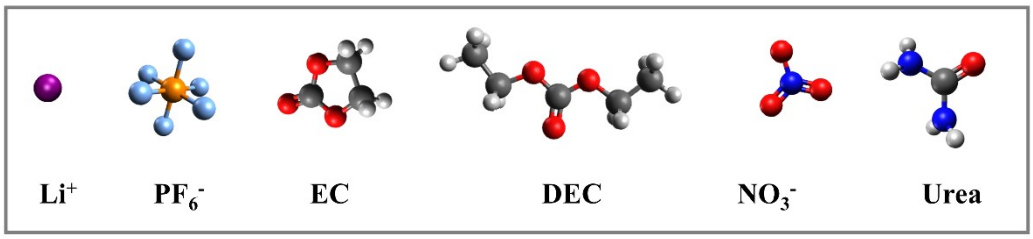

Fig. S17. Molecular structures of Li^+, PF_6^-, NO_3^-, ethylene carbonate (EC), diethyl carbonate (DEC), and urea used in Molecular Dynamics (MD) simulations. The color coding employed is purple (Li), orange (P), light blue (F), dark blue (N), red (O), gray (C), and white (H).

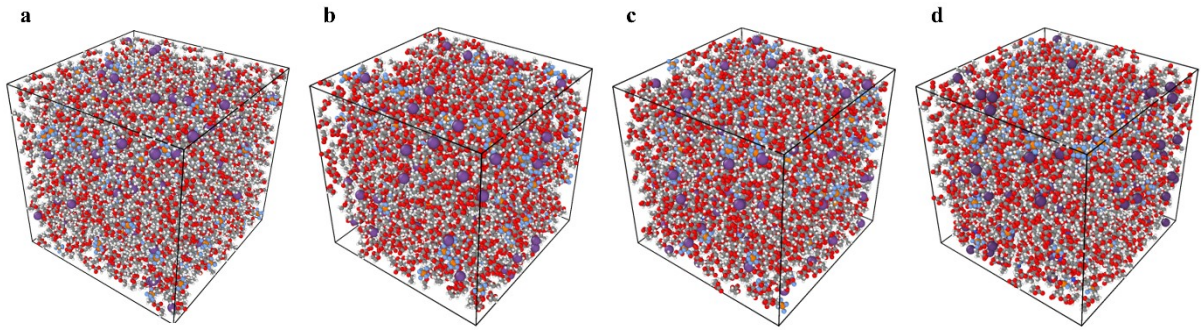

Fig. S18. Snapshots of 1.0 M $LiPF_6$ (a) in pure DEC (designated D), (b) in EC:DEC (1:1 v/v) (ED), (c) in EC:DEC (1:1 v/v) with 0.03 M $LiNO_3$ additive (EDN), and (d) in EC:DEC (1:1 v/v) with 0.03 M $LiNO_3$ additive and 0.1 M Urea co-additive (EDNU) electrolyte obtained by MD simulations. The color coding employed is purple (Li), orange (P), light blue (F), dark blue (N), red (O), gray (C), and white (H).

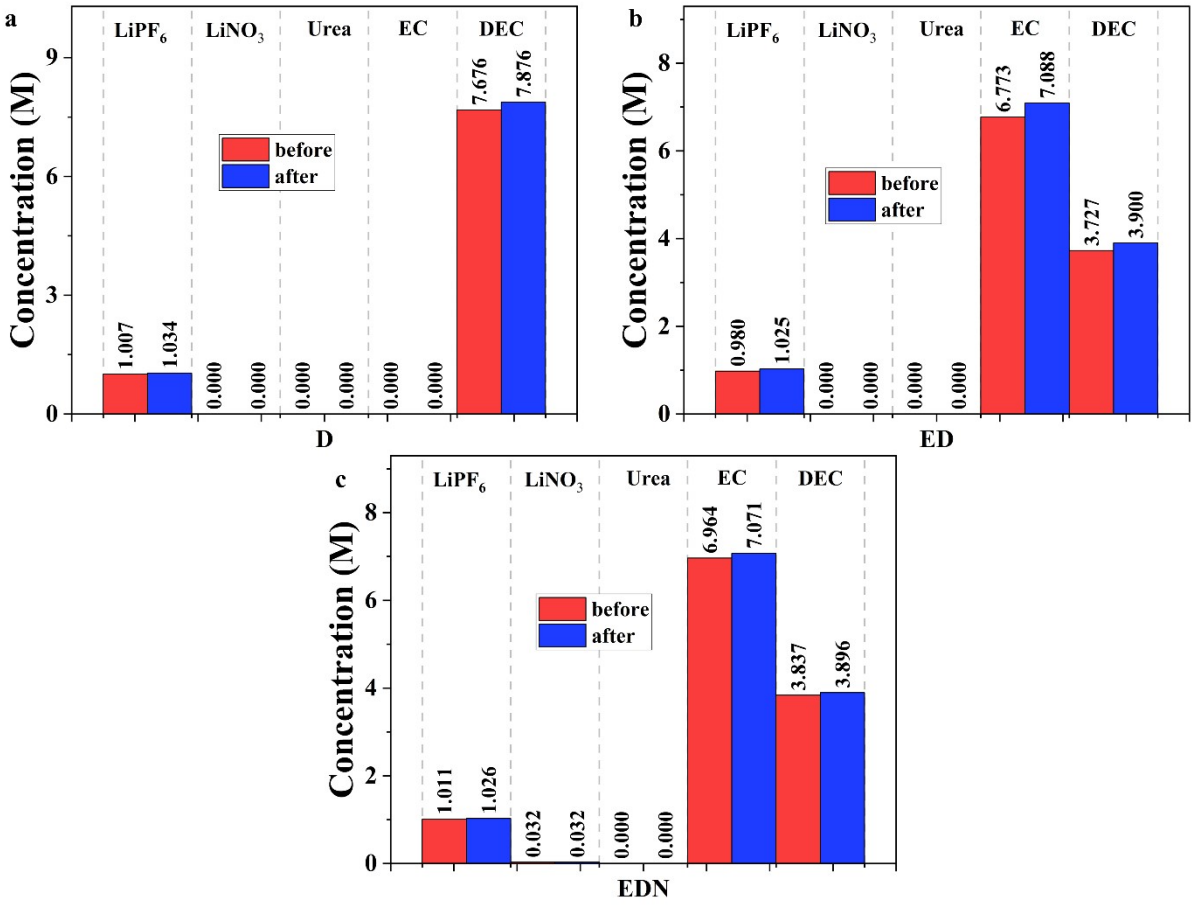

Fig. S19. The initial (before NPT equilibration) and final (post- NPT equilibration) concentrations for all systems: (a) D system, (b) ED, and (c) EDN.

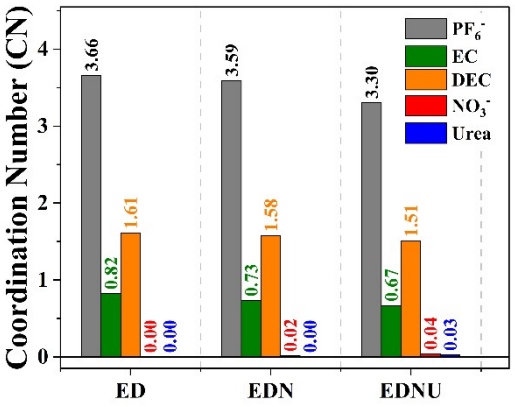

Fig. S20. Number of major coordinating species in the first Li^+ solvation shell.

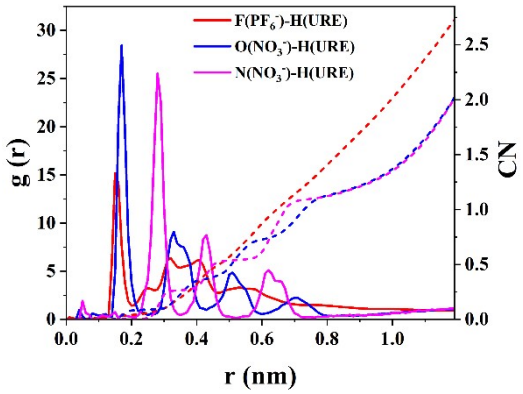

Fig. S21. Radial distribution function (RDF) and coordination number (CN) plots of F(PF_6^-)/O(NO_3^-)/ N(NO_3^-) and H(Urea) interactions

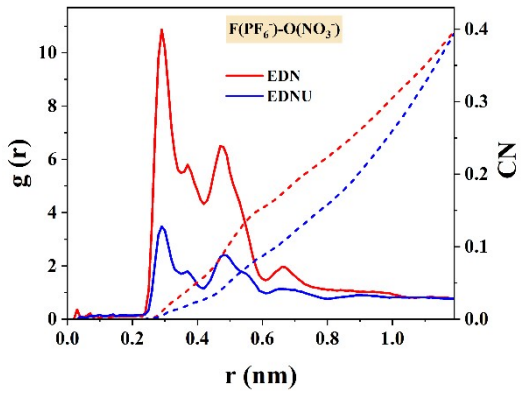

Fig. S22. Radial distribution function (RDF) and coordination number (CN) plots of F(PF_6^-)-O(NO_3^-) interactions.

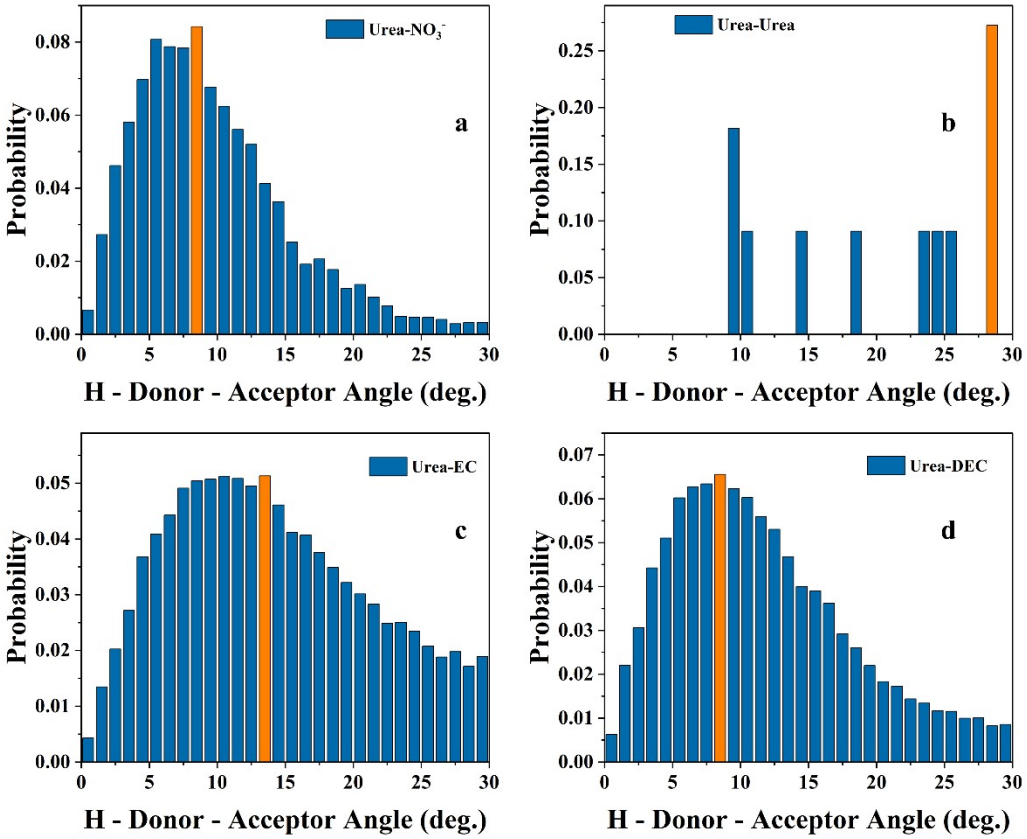

Fig. S23. Histograms of the distribution of angles of hydrogen bonds between urea and (a) nitrate anion, (b) urea, (c) EC, and (d) DEC species.

Table S1. Summary of UV-Vis baseline correction at 280 nm and analysis.

Description	Conc. (c) (M)	Absorbance at 280 nm (A_{280})	A_{net} ($A_{280}-A_{280,ED}$)
Base electrolyte (ED)	0	3.648	–
ED + 0.012 M $LiNO_3$ (EDN)	0.012	3.737	0.089
ED + 0.030 M $LiNO_3$ + 0.1 M Urea (EDNU)	0.030	3.890	0.242

Table S2. Comparative Li||Li symmetric cell performance and post-cycling resistance summary for EDNU cell.

Test Condition	Rate (mA cm^{-2}) / Cap. (mAh cm^{-2})	Lifetime (h)	Overpotential (mV)	R_s (Ω)	R_{SEI} (Ω)	R_{ct} (Ω)
Low Depth / Low Rate	0.5 / 1.0	1400	43	7.7	17.6	40.8
Low Depth / High Rate	1.0 / 1.0	650	99	8.9	52.1	47.7
High Depth / High Rate	1.0 / 3.0	213	207	6.1	44.5	223.3

Table S3. Comparison of the present EDNU system with a complementary urea + $LiNO_3$-based electrolyte study.

Category	**Wu et al. (**J. Mater. Chem. A 2024, 12, 15685–15692**)**	**This Work (EDNU Electrolyte)**	**Remarks / Novelty significance**
Baseline electrolyte	1 M $LiPF_6$ in DMC/FEC (2:1 v/v)	1 M $LiPF_6$ in EC/DEC (1:1 v/v)	Different solvent polarity and donor number; EC/DEC is more conventional and cost-effective. Demonstrating stable Li and NMC811 operation in EC/DEC is a key practical advance.
Additive composition	+ 0.05 M $LiNO_3$ + 0.1 M urea	+ 0.03 M $LiNO_3$ + 0.1 M urea	Lower $LiNO_3$ concentration (0.03 M), offering reduced cost and fewer parasitic reactions while maintaining stability.
Active electrodes	Li (50 µm) ‖ NCM811 (1.7 mAh cm^{-2})	Li (50 µm) ‖ NMC811 (1.5 mAh cm^{-2})	Similar cathode chemistry: comparable areal capacities enable qualitative comparison of interfacial behavior.
Cycling conditions	0.5 C (2.8–4.25 V)	1.5 C (2.8–4.25 V)	This work uses 3 times higher current density, testing the electrolyte under more demanding kinetics.
Full-cell performance	70.8 % capacity retention after 480 cycles	63.8 % capacity retention after 400 cycles (99.1 % avg CE; 0.09 % fade per cycle)	Despite harsher conditions and no FEC, the EC/DEC-based EDNU shows comparable long-term durability, confirming robust CEI formation and fast Li^+ transport.
Symmetric-cell lifetime	≈ 1300 h (0.5 mA cm^{-2}, 1.0 mAh cm^{-2})	≈ 1440 h (0.5 mA cm^{-2}, 1.0 mAh cm^{-2})	Both systems demonstrate long-term Li stability; EDNU matches or exceeds lifetime in a harsher EC/DEC medium.

Table S4. Summary of primary FTIR absorption bands observed on cycled NMC811 and the corresponding functional groups, vibrational modes, and the presumed role of each species in the CEI layer.

Wavenumber (cm-1)	Functional group / component	Vibrational mode	Source / Electrolyte where prominent	Assigned CEI species / role
3363	N–H stretching	Stretching	EDNU (strong)	Urea-derived N–H / hydrogen-bonded polymeric outer layer; promotes cohesion
2960 / 2870	C–H (alkyl)	Asymmetric/Symmetric stretching	All (weak–med)	Residual organic solvent or carbonate fragments
1823	Polycarbonate (PC) species	C=O stretching	EDNU (weak)	Minor EC/DEC oxidation product (suppressed in EDNU)
1767	Lithium alkyl carbonates / PC	C=O stretching	ED, EDN (strong)	Major solvent oxidation products ($ROCO_2Li$ / polycarbonate)
1640	Amide / urea derivative	N–C=O stretching	EDNU (strong)	Urea decomposition, N-rich polymeric CEI (outer layer)
1420	C–H bending	Bending / asymmetric C–O stretching	All (medium)	Inorganic carbonate species (Li_2CO_3)
1303	N-oxide / NO_x species	Stretching	EDNU (strong)	Products from $LiNO_3$ reduction (N-containing inorganic species)
1183	Polyether / PC	C–O stretching	ED, EDN (strong)	Polymerized solvent fragments; diminished in EDNU
1059	Phosphorus–oxygen (P–O)	P–O stretching	All (strong)	$Li_xPO_yF_z$ / lithium fluorophosphate species (inorganic inner CEI)
837	Phosphorus–fluorine (P–F) / Li–F	P–F /Li–F stretching	All (strong)	LiF / $Li_xPO_yF_z$, inorganic, Li^+-conductive inner layer

Table S5. Interfacial composition summary of the cycled NMC811 cells

Electrolyte	Surface N (at%)	Surface C/F Ratio	Inner F (at%)	Inner N (at%)
ED	0.00	1.12	21.26	0.00
EDN	0.43	1.43	33.19	0.41
EDNU	0.87	0.88	36.62	0.42

Table S6. Densities comparison of pure diethyl carbonate (DEC), and a 1:1 volume ratio mixture of EC: DEC (ED), all containing 1.0 M $LiPF_6$ salt.

System	Density (g cm^{-3})		Deviation (%)
	Experimental	MD Simulated	
D (1.0 M $LiPF_6$ in pure DEC)	1.090	1.088	-0.17
ED (1.0 M $LiPF_6$ in EC:DEC (1:1 v/v))	1.260	1.240	-1.57

Table S7. Radial distribution function (RDF) and coordination number (CN) data for key interactions in the first solvation shells of the electrolytes.

System	Interaction pair	r_max(nm)	g(r)_max	r_min (nm)	CN
ED	Li^+-F(PF_6)	0.19	83.10	0.26	3.66
	Li^+-O(EC)	0.21	2.75	0.30	0.82
	Li^+-O(DEC)	0.20	14.63	0.31	1.61
EDN	Li^+-F(PF_6)	0.19	82.95	0.26	3.59
	Li^+-O(EC)	0.21	2.12	0.30	0.73
	Li^+-O(DEC)	0.20	13.74	0.31	1.58
	Li^+-O(NO_3)	0.20	54.55	0.27	0.02
	Li^+-N(NO_3)	0.24	31.28	0.27	0.004
	F(PF_6)-O(NO_3)	0.29	10.87	0.35	0.033
	F(PF_6)-N(NO_3)	0.35	15.13	0.47	0.050
EDNU	Li^+-F(PF_6)	0.19	76.97	0.26	3.30
	Li^+-O(EC)	0.21	1.81	0.30	0.67
	Li^+-O(DEC)	0.20	13.30	0.31	1.51
	Li^+-O(NO_3)	0.20	123.88	0.26	0.04
	Li^+-N(NO_3)	0.29	71.89	0.38	0.032
	F(PF_6)-O(NO_3)	0.30	3.48	0.35	0.016
	F(PF_6)-N(NO_3)	0.36	4.17	0.47	0.014
	Li^+-O(URE)	0.32	19.25	0.38	0.025
	Li^+-N(URE)	0.20	86.38	0.29	0.041
	O(EC)-H(URE)	0.18	0.54	0.24	0.003
	O(DEC)-H(URE)	0.17	1.73	0.25	0.008
	O(EC)-N(URE)	0.28	0.58	0.34	0.005
	O(DEC)-N(URE)	0.27	1.6	0.37	0.013
	F(PF_6)-H(URE)	0.15	15.21	0.20	0.041
	O(NO_3)-H(URE)	0.17	28.43	0.25	0.090
	N(NO_3)-H(URE)	0.28	25.30	0.35	0.266

Table S8. Residence time analysis for key interactions in the first solvation shells.

System	Residence time (ns)				
	PF_6^-	EC	DEC	NO_3^-	Urea
ED	7.98	8.97	9.45	-	-
EDN	6.51	6.39	11.69	7.37	-
EDNU	5.05	3.77	4.99	10.28	5.79

Force field data of EC, DEC, PF6-, NO3-, and Urea

EC:

[moleculetype]

; Name nrexcl

EC 3

[atoms]

; nr type resnr residue atom cgnr charge mass

1 opls_820 1 EC O00 1 -0.4167 15.9990

2 opls_819 1 EC C01 1 0.5330 12.0110

3 opls_821 1 EC O02 1 -0.2778 15.9990

4 opls_822 1 EC C03 1 -0.0455 12.0110

5 opls_823 1 EC C04 1 -0.0453 12.0110

6 opls_824 1 EC O05 1 -0.2777 15.9990

7 opls_825 1 EC H06 1 0.1325 1.0080

8 opls_826 1 EC H07 1 0.1325 1.0080

9 opls_827 1 EC H08 1 0.1325 1.0080

10 opls_828 1 EC H09 1 0.1325 1.0080

[bonds]

; ai aj funct c0 c1

1 2 1 0.1229 476976.000

3 2 1 0.1327 179075.200

4 3 1 0.1410 267776.000

5 4 1 0.1529 224262.400

6 5 1 0.1410 267776.000

7 4 1 0.1090 284512.000

8 4 1 0.1090 284512.000

9 5 1 0.1090 284512.000

10 5 1 0.1090 284512.000

6 2 1 0.1327 179075.200

[angles]

; ai	aj	ak	funct	c0	c1
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4	3	2	1	116.900	694.544
5	4	3	1	109.500	418.400
6	5	4	1	109.500	418.400
7	4	3	1	109.500	292.880
8	4	3	1	109.500	292.880
9	5	4	1	110.700	313.800
10	5	4	1	110.700	313.800
6	2	1	1	123.400	694.544
6	2	3	1	117.450	586.848
7	4	5	1	110.700	313.800
8	4	5	1	110.700	313.800
9	5	6	1	109.500	292.880
10	5	6	1	109.500	292.880
8	4	7	1	107.800	276.144
10	5	9	1	107.800	276.144
5	6	2	1	116.900	694.544

[dihedrals]

; PROPER DIHEDRAL ANGLES

; ai	aj	ak	al	funct	c0	c1	c2	c3	c4	c5
4	3	2	1	3	21.439	0.000	-21.439	-0.000	-0.000	0.000
5	4	3	2	3	-2.197	5.201	0.527	-3.531	-0.000	0.000
6	5	4	3	3	-1.151	1.151	0.000	-0.000	-0.000	0.000
7	4	3	2	3	0.414	1.243	0.000	-1.657	-0.000	0.000
8	4	3	2	3	0.414	1.243	0.000	-1.657	-0.000	0.000
9	5	4	3	3	0.628	1.883	0.000	-2.510	-0.000	0.000
10	5	4	3	3	0.628	1.883	0.000	-2.510	-0.000	0.000
5	6	2	1	3	21.439	0.000	-21.439	-0.000	-0.000	0.000
5	6	2	3	3	31.206	-9.768	-21.439	-0.000	-0.000	0.000
6	2	3	4	3	31.206	-9.768	-21.439	-0.000	-0.000	0.000

```
   7    4    5    6    3      0.628   1.883    0.000  -2.510  -0.000   0.000
   8    4    5    6    3      0.628   1.883    0.000  -2.510  -0.000   0.000
   9    5    4    7    3      0.628   1.883    0.000  -2.510  -0.000   0.000
  10    5    4    7    3      0.628   1.883    0.000  -2.510  -0.000   0.000
   9    5    4    8    3      0.628   1.883    0.000  -2.510  -0.000   0.000
  10    5    4    8    3      0.628   1.883    0.000  -2.510  -0.000   0.000
   2    6    5    9    3      0.414   1.243    0.000  -1.657  -0.000   0.000
   2    6    5   10    3      0.414   1.243    0.000  -1.657  -0.000   0.000
   4    5    6    2    3     -2.197   5.201    0.527  -3.531  -0.000   0.000

[ dihedrals ]
;IMPROPER DIHEDRAL ANGLES
;  ai    aj   ak   al funct      c0       c1      c2      c3      c4      c5
   1    2    3    6    4     180.000   43.932      2
[ pairs ]
;  ai    aj funct
   2    7    1
   2    8    1
   2    9    1
   2   10    1
   1    4    1
   1    5    1
   3    9    1
   3   10    1
   6    7    1
   6    8    1
   7    9    1
   7   10    1
   8    9    1
   8   10    1
```

DEC:

```
[ moleculetype ]
```

; Name nrexcl

DEC 3

[atoms]

; nr type resnr residue atom cgnr charge mass

1 opls_808 1 DEC H10 1 0.1035 1.0080

2 opls_807 1 DEC C5 1 -0.2478 12.0110

3 opls_809 1 DEC H8 1 0.1035 1.0080

4 opls_810 1 DEC H9 1 0.1035 1.0080

5 opls_806 1 DEC C4 1 0.0296 12.0110

6 opls_811 1 DEC H6 1 0.1071 1.0080

7 opls_812 1 DEC H7 1 0.1071 1.0080

8 opls_801 1 DEC O3 1 -0.3390 15.9990

9 opls_800 1 DEC C3 1 0.5800 12.0110

10 opls_802 1 DEC O2 1 -0.5148 15.9990

11 opls_803 1 DEC O1 1 -0.3390 15.9990

12 opls_804 1 DEC C2 1 0.0296 12.0110

13 opls_813 1 DEC H4 1 0.1071 1.0080

14 opls_814 1 DEC H5 1 0.1071 1.0080

15 opls_805 1 DEC C1 1 -0.2479 12.0110

16 opls_815 1 DEC H1 1 0.1035 1.0080

17 opls_816 1 DEC H2 1 0.1035 1.0080

18 opls_817 1 DEC H3 1 0.1034 1.0080

[bonds]

; ai aj funct c0 c1

8 9 1 0.1327 179075.200

10 9 1 0.1229 476976.000

11 9 1 0.1327 179075.200

12 11 1 0.1410 267776.000

15 12 1 0.1529 224262.400

5 8 1 0.1410 267776.000

2 5 1 0.1529 224262.400

```
  1    2    1      0.1090    284512.000
  3    2    1      0.1090    284512.000
  4    2    1      0.1090    284512.000
  6    5    1      0.1090    284512.000
  7    5    1      0.1090    284512.000
 13   12    1      0.1090    284512.000
 14   12    1      0.1090    284512.000
 16   15    1      0.1090    284512.000
 17   15    1      0.1090    284512.000
 18   15    1      0.1090    284512.000

[angles]
;  ai    aj    ak  funct      c0       c1
   10    9     8    1       123.400    694.544
   11    9     8    1       117.450    586.848
   12   11     9    1       116.900    694.544
   15   12    11    1       109.500    418.400
    5    8     9    1       116.900    694.544
    2    5     8    1       109.500    418.400
    1    2     5    1       110.700    313.800
    3    2     5    1       110.700    313.800
    4    2     5    1       110.700    313.800
    6    5     8    1       109.500    292.880
    7    5     8    1       109.500    292.880
   13   12    11    1       109.500    292.880
   14   12    11    1       109.500    292.880
   16   15    12    1       110.700    313.800
   17   15    12    1       110.700    313.800
   18   15    12    1       110.700    313.800
   11    9    10    1       123.400    694.544
   13   12    15    1       110.700    313.800
   14   12    15    1       110.700    313.800
    6    5    2     1       110.700    313.800
```

```
   7    5    2    1      110.700    313.800
   3    2    1    1      107.800    276.144
   4    2    1    1      107.800    276.144
   4    2    3    1      107.800    276.144
   7    5    6    1      107.800    276.144
  14   12   13    1      107.800    276.144
  17   15   16    1      107.800    276.144
  18   15   16    1      107.800    276.144
  18   15   17    1      107.800    276.144

[ dihedrals ]
;  PROPER DIHEDRAL ANGLES
;  ai    aj   ak   al funct      c0       c1      c2      c3      c4     c5
   12   11    9    8    3     31.206  -9.768  -21.439  -0.000  -0.000   0.000
   15   12   11    9    3     -2.197   5.201    0.527  -3.531  -0.000   0.000
    5    8    9   10    3     21.439   0.000  -21.439  -0.000  -0.000   0.000
    2    5    8    9    3     -2.197   5.201    0.527  -3.531  -0.000   0.000
    1    2    5    8    3      0.628   1.883    0.000  -2.510  -0.000   0.000
    3    2    5    8    3      0.628   1.883    0.000  -2.510  -0.000   0.000
    4    2    5    8    3      0.628   1.883    0.000  -2.510  -0.000   0.000
    6    5    8    9    3      0.414   1.243    0.000  -1.657  -0.000   0.000
    7    5    8    9    3      0.414   1.243    0.000  -1.657  -0.000   0.000
   13   12   11    9    3      0.414   1.243    0.000  -1.657  -0.000   0.000
   14   12   11    9    3      0.414   1.243    0.000  -1.657  -0.000   0.000
   16   15   12   11    3      0.628   1.883    0.000  -2.510  -0.000   0.000
   17   15   12   11    3      0.628   1.883    0.000  -2.510  -0.000   0.000
   18   15   12   11    3      0.628   1.883    0.000  -2.510  -0.000   0.000
   12   11    9   10    3     21.439   0.000  -21.439  -0.000  -0.000   0.000
    5    8    9   11    3     31.206  -9.768  -21.439  -0.000  -0.000   0.000
    6    5    2    1    3      0.628   1.883    0.000  -2.510  -0.000   0.000
    7    5    2    1    3      0.628   1.883    0.000  -2.510  -0.000   0.000
    6    5    2    3    3      0.628   1.883    0.000  -2.510  -0.000   0.000
    7    5    2    3    3      0.628   1.883    0.000  -2.510  -0.000   0.000
```

```
   6    5    2    4    3      0.628   1.883    0.000  -2.510  -0.000   0.000
   7    5    2    4    3      0.628   1.883    0.000  -2.510  -0.000   0.000
  16   15   12   13    3      0.628   1.883    0.000  -2.510  -0.000   0.000
  17   15   12   13    3      0.628   1.883    0.000  -2.510  -0.000   0.000
  18   15   12   13    3      0.628   1.883    0.000  -2.510  -0.000   0.000
  16   15   12   14    3      0.628   1.883    0.000  -2.510  -0.000   0.000
  17   15   12   14    3      0.628   1.883    0.000  -2.510  -0.000   0.000
  18   15   12   14    3      0.628   1.883    0.000  -2.510  -0.000   0.000

[ dihedrals ]
;IMPROPER DIHEDRAL ANGLES
;  ai    aj   ak   al funct      c0       c1      c2      c3      c4      c5
   8    9   10   11     4     180.000   43.932       2
[ pairs ]
;  ai    aj funct
   9   15    1
   9    2    1
   9    6    1
   9    7    1
   9   13    1
   9   14    1
   8   12    1
   8    1    1
   8    3    1
   8    4    1
  10   12    1
  10    5    1
  11    5    1
  11   16    1
  11   17    1
  11   18    1
   1    6    1
   1    7    1
```

3 6 1

3 7 1

4 6 1

4 7 1

13 16 1

13 17 1

13 18 1

14 16 1

14 17 1

14 18 1

PF_6^-:

[moleculetype]

; Name nrexcl

PF6 3

[atoms]

; nr type resnr residue atom cgnr charge mass

1 opls_835 1 PF6 P1 1 2.8809 30.9740

2 opls_836 1 PF6 F1 1 -0.6468 18.9980

3 opls_837 1 PF6 F2 1 -0.6468 18.9980

4 opls_838 1 PF6 F3 1 -0.6468 18.9980

5 opls_839 1 PF6 F4 1 -0.6468 18.9980

6 opls_840 1 PF6 F5 1 -0.6468 18.9980

7 opls_841 1 PF6 F6 1 -0.6469 18.9980

[bonds]

; ai aj funct c0 c1

2 1 1 0.1550 256412.256

3 1 1 0.1550 256412.256

4 1 1 0.1550 256412.256

5 1 1 0.1550 256412.256

6 1 1 0.1550 256412.256

7 1 1 0.1550 256412.256

[angles]

; ai aj ak funct c0 c1

3 1 2 1 108.400 531.954

4 1 2 1 108.400 531.954

5 1 2 1 108.400 531.954

6 1 2 1 108.400 531.954

7 1 2 1 108.400 531.954

4 1 3 1 108.400 531.954

5 1 3 1 108.400 531.954

6 1 3 1 108.400 531.954

7 1 3 1 108.400 531.954

5 1 4 1 108.400 531.954

6 1 4 1 108.400 531.954

7 1 4 1 108.400 531.954

6 1 5 1 108.400 531.954

7 1 5 1 108.400 531.954

7 1 6 1 108.400 531.954

[dihedrals]

; PROPER DIHEDRAL ANGLES

; ai aj ak al funct c0 c1 c2 c3 c4 c5

[dihedrals]

;IMPROPER DIHEDRAL ANGLES

; ai aj ak al funct c0 c1 c2 c3 c4 c5

[pairs]

; ai aj funct

NO_3^-:

[moleculetype]

```
; Name            nrexcl
  NO3               3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass
     1   opls_831      1    NO3    O3      1    -0.6068    15.9990
     2   opls_830      1    NO3    N1      1     0.8204    14.0070
     3   opls_832      1    NO3    O1      1    -0.6068    15.9990
     4   opls_833      1    NO3    O2      1    -0.6068    15.9990

[ bonds ]
;  ai    aj   funct      c0       c1
    1    2    1      0.1225    460240.000
    3    2    1      0.1225    460240.000
    4    2    1      0.1225    460240.000

[angles]
;  ai    aj   ak  funct      c0       c1
    3    2    1    1       125.000    669.440
    4    2    1    1       125.000    669.440
    4    2    3    1       125.000    669.440

[ dihedrals ]
;  PROPER DIHEDRAL ANGLES
;  ai    aj   ak   al funct      c0       c1      c2      c3      c4      c5

[ dihedrals ]
;IMPROPER DIHEDRAL ANGLES
;  ai    aj   ak   al funct      c0       c1      c2      c3      c4      c5
    1    2    3    4     4     180.000   10.460      2
[ pairs ]
;  ai    aj funct
```

Urea:

```
[ moleculetype ]
; Name            nrexcl
  URE               3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass
     1   opls_853     1    URE   C00      1     1.0054    12.0110
     2   opls_854     1    URE   O01      1    -0.3982    15.9990
     3   opls_855     1    URE   N02      1    -1.4504    14.0070
     4   opls_856     1    URE   N03      1    -1.4736    14.0070
     5   opls_857     1    URE   H04      1     0.5773     1.0080
     6   opls_858     1    URE   H05      1     0.5773     1.0080
     7   opls_859     1    URE   H06      1     0.5811     1.0080
     8   opls_860     1    URE   H07      1     0.5811     1.0080

[ bonds ]
;  ai    aj   funct      c0       c1
    2    1    1      0.1229    476976.000
    3    1    1      0.1335    410032.000
    4    1    1      0.1335    410032.000
    5    3    1      0.1010    363171.200
    6    3    1      0.1010    363171.200
    7    4    1      0.1010    363171.200
    8    4    1      0.1010    363171.200

[angles]
;  ai    aj   ak  funct      c0       c1
    3    1    2    1       122.900    669.440
    4    1    2    1       122.900    669.440
    5    3    1    1       119.800    292.880
    6    3    1    1       119.800    292.880
    7    4    1    1       119.800    292.880
```

```
   8   4   1   1      119.800   292.880
   4   1   3   1      114.200   585.760
   6   3   5   1      120.000   292.880
   8   4   7   1      120.000   292.880
[ dihedrals ]
;  PROPER DIHEDRAL ANGLES
;  ai    aj   ak   al funct      c0       c1      c2      c3      c4      c5
   5   3   1   2   3     20.502   0.000  -20.502  -0.000  -0.000   0.000
   6   3   1   2   3     20.502   0.000  -20.502  -0.000  -0.000   0.000
   7   4   1   2   3     20.502   0.000  -20.502  -0.000  -0.000   0.000
   8   4   1   2   3     20.502   0.000  -20.502  -0.000  -0.000   0.000
   7   4   1   3   3     20.502   0.000  -20.502  -0.000  -0.000   0.000
   8   4   1   3   3     20.502   0.000  -20.502  -0.000  -0.000   0.000
   5   3   1   4   3     20.502   0.000  -20.502  -0.000  -0.000   0.000
   6   3   1   4   3     20.502   0.000  -20.502  -0.000  -0.000   0.000
[ dihedrals ]
;IMPROPER DIHEDRAL ANGLES
;  ai    aj   ak   al funct      c0       c1      c2      c3      c4      c5
   2   1   3   4    4    180.000   43.932      2
   1   3   5   6    4    180.000   10.460      2
   1   4   7   8    4    180.000   10.460      2
[ pairs ]
;  ai    aj funct
   2   5   1
   2   6   1
   2   7   1
   2   8   1
   3   7   1
   3   8   1
   4   5   1
   4   6   1
```