Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY MATERIALS

I. Measured volumetric data

Table S1: Density (ρ, g/cm^{-3}) dependence on LiCl concentration (m, mol/kg) and temperature.

	ρ				
m	**308 K**	**313 K**	**318 K**	**323 K**	**328 K**
0	0.94564	0.94145	0.93726	0.93306	0.92888
0.01418	0.94596	0.94177	0.93759	0.93341	0.92923
0.02183	0.94613	0.94195	0.93776	0.93359	0.92942
0.03418	0.94650	0.94231	0.93813	0.93395	0.92978
0.04628	0.94676	0.94257	0.93839	0.93422	0.93006
0.06371	0.94734	0.94316	0.93899	0.93482	0.93066
0.08235	0.94783	0.94366	0.93949	0.93533	0.93117
0.10567	0.94843	0.94427	0.94010	0.93595	0.93180
0.12684	0.94898	0.94482	0.94066	0.93651	0.93237
0.16690	0.95000	0.94584	0.94170	0.93756	0.93343
0.19020	0.95068	0.94654	0.94240	0.93827	0.93414
0.30548	0.95369	0.94957	0.94546	0.94136	0.93726
0.40664	0.95636	0.95227	0.94819	0.94411	0.94005

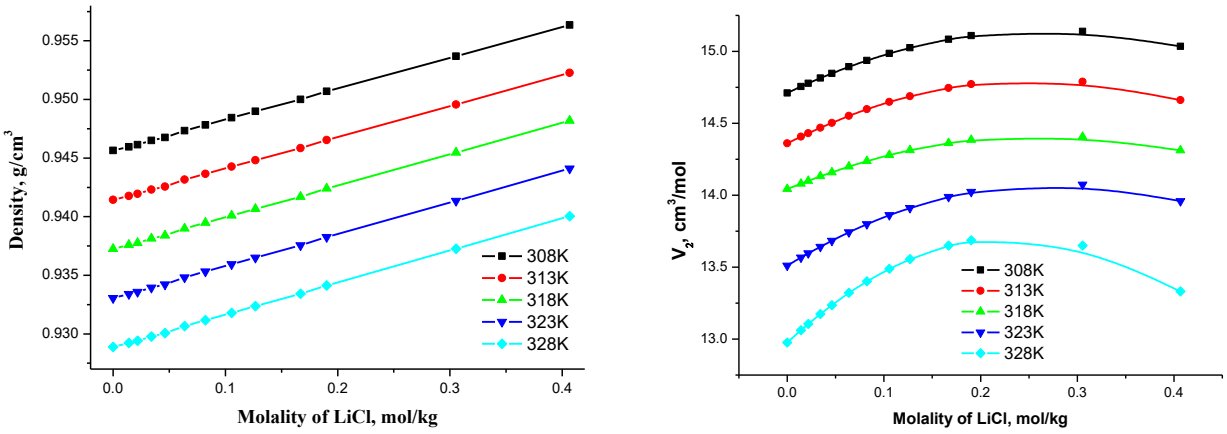

Figure S1: Density and partial molar volume dependence on LiCl concentration and temperature.

II. DFT energetic calculations.

Table S2: Thermodynamic functions of $Cl(NMA)_x^-$ complex formation in different functionals and NMA stoichiometry. All values are expressed in $kcal.mol^{-1}$ and θ refers to 1 mol, 298.15 K and 1 bar standard conditions.

$\Delta_R E$								
NMA	**PBE**	**BLYP**	**PW91**	**TPSS**	**B3LYP**	**B3PW91**	**BMK**	**M06**
1	-22.7	-20.2	-23.2	-21.4	-20.7	-20.7	-21.0	-23.1
2	-40.4	-36.1	-41.3	-38.2	-37.3	-37.0	-38.1	-41.8
3	-54.5	-48.7	-55.7	-51.5	-50.7	-49.9	-52.1	-57.0
4	-66.0	-58.1	-67.9	-62.2	-62.8	-59.5	-62.5	[a]

$\Delta_R H^0$								
NMA	**PBE**	**BLYP**	**PW91**	**TPSS**	**B3LYP**	**B3PW91**	**BMK**	**M06**
1	-22.9	-20.2	-23.4	-21.5	-20.6	-20.7	-20.9	-22.4
2	-39.4	-34.8	-40.3	-37.1	-35.9	-35.7	-36.5	-39.1
3	-52.1	-46.1	-53.3	-49.0	-48.0	-47.3	-48.9	-52.4
4	-62.8	-54.1	-64.7	-58.8	-58.7	-55.6	-57.8	[a]

$\Delta_R G^0$								
NMA	**PBE**	**BLYP**	**PW91**	**TPSS**	**B3LYP**	**B3PW91**	**BMK**	**M06**
1	-15.9	-13.0	-16.3	-14.5	-13.0	-13.4	-15.0	-16.1
2	-25.7	-20.5	-26.3	-23.0	-20.8	-21.4	-21.8	-25.4
3	-30.4	-23.5	-31.7	-27.0	-23.9	-24.3	-24.6	-31.6
4	-31.3	-23.3	-32.2	-25.3	-26.5	-25.6	-25.6	[a]

$-T\Delta_R S^0$								
NMA	**PBE**	**BLYP**	**PW91**	**TPSS**	**B3LYP**	**B3PW91**	**BMK**	**M06**
1	7.0	7.2	7.1	7.0	7.6	7.3	5.9	6.3
2	13.7	14.3	14.0	14.1	15.2	14.3	14.7	13.7
3	21.8	22.5	21.6	22.0	24.0	23.0	24.3	20.8
4	31.6	30.8	32.5	33.5	32.2	30.0	32.2	[a]

a complex $Cl(NMA)_4^-$ did not converge in M06 functional.

Table S3: Thermodynamic functions of $Li(NMA)_x^+$ complex formation in different functionals and NMA stoichiometry. All values are expressed in $kcal.mol^{-1}$ and θ refers to 1 mol, 298.15 K and 1 bar standard conditions.

$\Delta_R E$								
NMA	**PBE**	**BLYP**	**PW91**	**TPSS**	**B3LYP**	**B3PW91**	**BMK**	**M06**
1	-55.6	-56.3	-56.3	-55.8	-57.5	-55.2	-55.0	-54.6
2	-96.2	-97.0	-97.5	-96.4	-99.5	-95.5	-95.0	-94.5
3	-119.2	-118.9	-120.9	-118.8	-122.5	-117.2	-117.2	-117.9
4	-134.0	-130.0	-136.3	-131.9	-135.4	-128.9	-132.0	-138.9

$\Delta_R H^0$								
NMA	**PBE**	**BLYP**	**PW91**	**TPSS**	**B3LYP**	**B3PW91**	**BMK**	**M06**
1	-54.3	-55.0	-55.0	-55.1	-56.3	-54.0	-53.8	-52.9
2	-93.1	-93.9	-94.4	-93.3	-96.4	-92.5	-92.0	-91.1
3	-114.6	-114.3	-116.2	-114.2	-118.0	-113.4	-113.3	-111.7
4	-128.1	-124.0	-130.4	-126.0	-129.6	-123.1	-125.8	-130.4

$\Delta_R G^0$								
NMA	**PBE**	**BLYP**	**PW91**	**TPSS**	**B3LYP**	**B3PW91**	**BMK**	**M06**
1	-47.1	-47.3	-47.8	-46.1	-48.0	-46.2	-46.3	-45.8
2	-77.3	-77.3	-78.3	-77.5	-78.9	-75.9	-77.3	-74.2
3	-90.8	-89.4	-92.2	-89.7	-91.8	-87.4	-87.1	-87.1
4	-90.9	-86.8	-93.1	-89.1	-90.5	-85.3	-84.8	-90.4

$-T\Delta_R S^0$								
NMA	**PBE**	**BLYP**	**PW91**	**TPSS**	**B3LYP**	**B3PW91**	**BMK**	**M06**
1	7.2	7.7	7.2	9.0	8.3	7.8	7.5	7.1
2	15.8	16.6	16.0	15.7	17.5	16.6	14.7	17.0
3	23.8	24.9	24.0	24.4	26.3	26.1	26.2	24.6
4	37.2	37.3	37.3	36.9	39.1	37.8	41.0	39.9

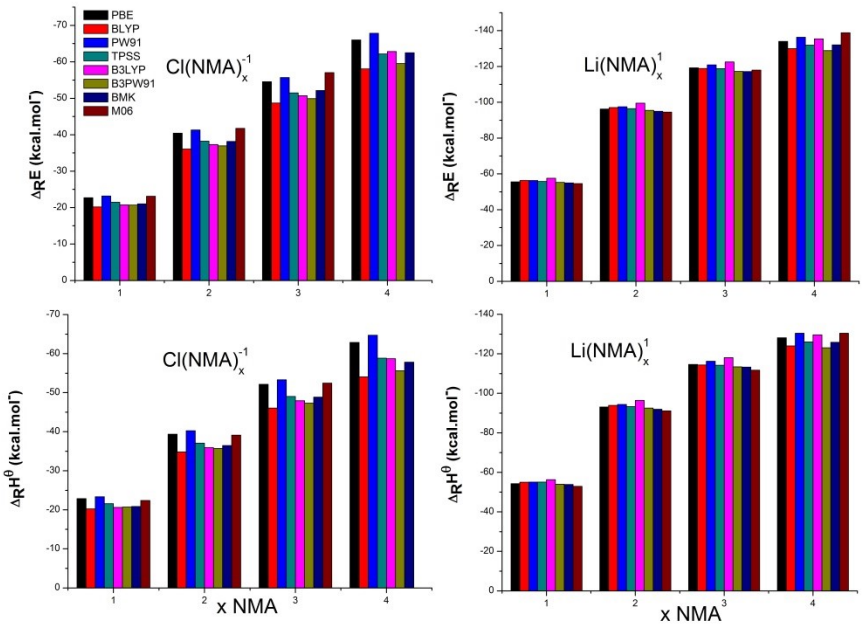

Figure S2: Variations of reaction electronic energies ($\Delta_R E$) and enthalpies ($\Delta_R H^\theta$) for $Cl(NMA)_x^-$ and $Li(NMA)_x^+$ complex formation on different functionals and NMA stoichiometry.

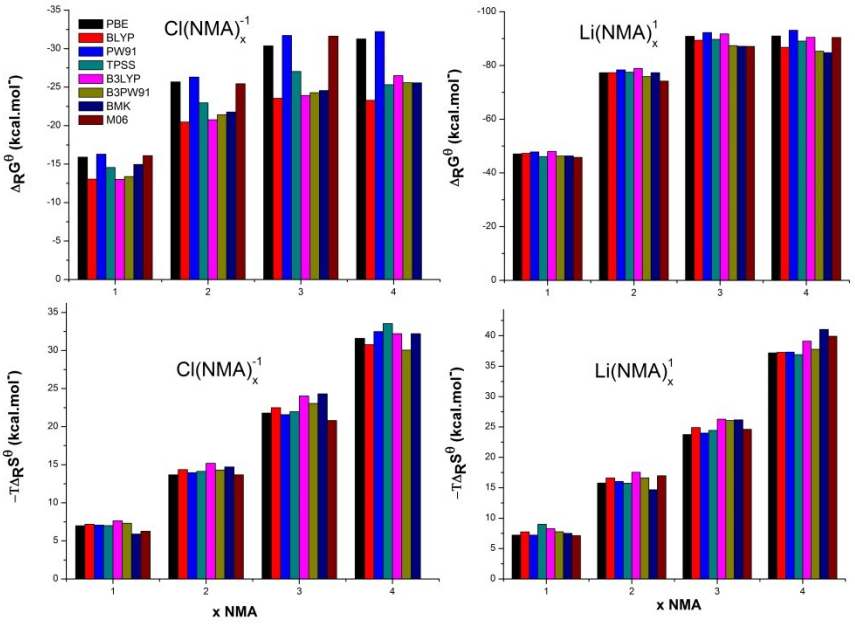

Figure S3: Variations of reaction Gibbs' free energies ($\Delta_R G$) and entropic term ($-T\Delta_R S^\theta$) for $Cl(NMA)_x^-$ and $Li(NMA)_x^+$ complex formation on different functionals and NMA stoichiometry.

Table S4: Total thermodynamic functions of LiCl-$(NMA)_x$ complex formation in different functionals and NMA stoichiometry. All values are expressed in kcal.mol^{-1} and θ refers to 1 mol, 298.15 K and 1 bar standard conditions.

$\Delta_R E$								
NMA	**PBE**	**BLYP**	**PW91**	**TPSS**	**B3LYP**	**B3PW91**	**BMK**	**M06**
1	-78.3	-76.5	-79.5	-77.2	-78.3	-75.9	-76.0	-77.7
2	-136.6	-133.1	-138.8	-134.6	-136.8	-132.5	-133.1	-136.3
3	-173.7	-167.6	-176.5	-170.3	-173.2	-167.2	-169.3	-175.0
4	-200.0	-188.1	-204.1	-194.0	-198.3	-188.4	-194.5	[a]

$\Delta_R H^0$								
NMA	**PBE**	**BLYP**	**PW91**	**TPSS**	**B3LYP**	**B3PW91**	**BMK**	**M06**
1	-77.2	-75.2	-78.4	-76.6	-76.9	-74.7	-74.7	-75.3
2	-132.4	-128.7	-134.6	-130.3	-132.4	-128.2	-128.4	-130.2
3	-166.7	-160.4	-169.5	-163.2	-166.0	-160.8	-162.2	-164.1
4	-191.0	-178.1	-195.1	-184.8	-188.3	-178.7	-183.6	[a]

$\Delta_R G^0$								
NMA	**PBE**	**BLYP**	**PW91**	**TPSS**	**B3LYP**	**B3PW91**	**BMK**	**M06**
1	-63.0	-60.3	-64.1	-60.6	-61.0	-59.6	-61.3	-61.9
2	-103.0	-97.7	-104.6	-100.5	-99.6	-97.3	-99.1	-99.6
3	-121.2	-113.0	-124.0	-116.8	-115.7	-111.6	-111.7	-118.7
4	-122.2	-110.1	-125.3	-114.4	-117.0	-110.9	-110.3	[a]

$-T\Delta_R S^0$								
NMA	**PBE**	**BLYP**	**PW91**	**TPSS**	**B3LYP**	**B3PW91**	**BMK**	**M06**
1	14.2	14.9	14.3	16.0	15.9	15.1	13.4	13.4
2	29.4	31.0	30.0	29.9	32.7	30.9	29.4	30.6
3	45.5	47.4	45.6	46.4	50.3	49.1	50.5	45.4
4	68.8	68.0	69.8	70.4	71.3	67.8	73.3	[a]

a complex $Cl(NMA)_4^-$ did not converge in M06 functional.

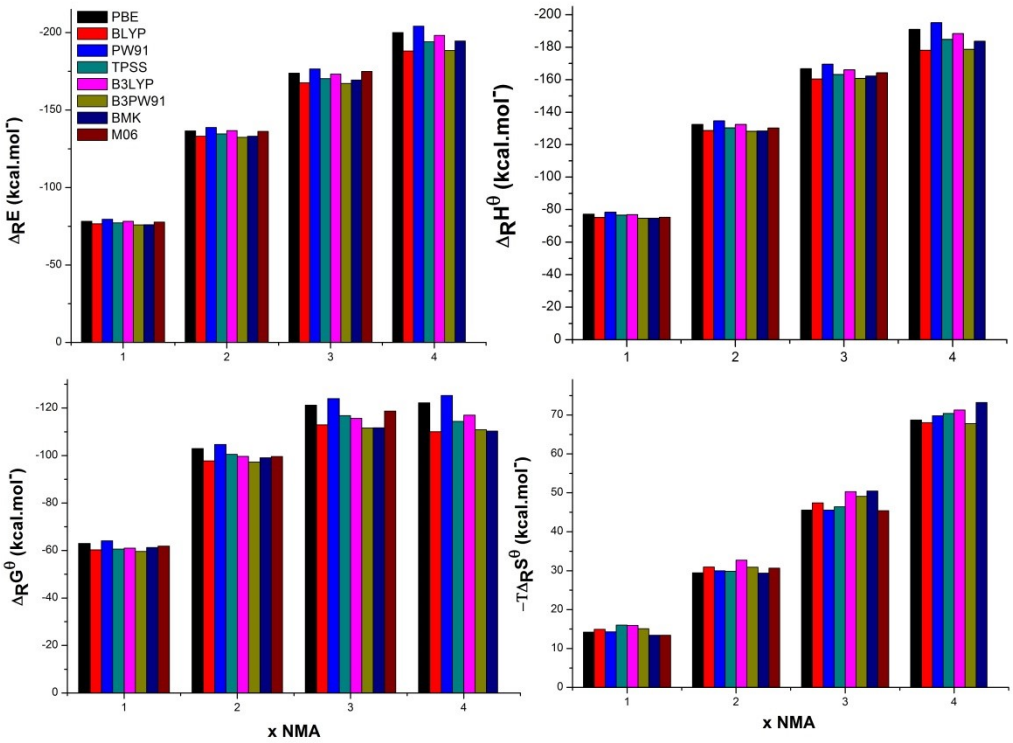

Figure S4: Variations of thermodynamic function to $Cl(NMA)_x^-$ and $Li(NMA)_x^+$ complex formation together on different functionals and NMA stoichiometry

III. Structural Parameters

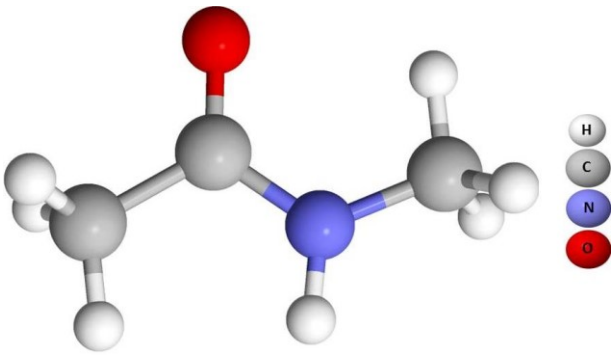

Figure S5: n-methylacetamide (NMA) equilibrium geometry.

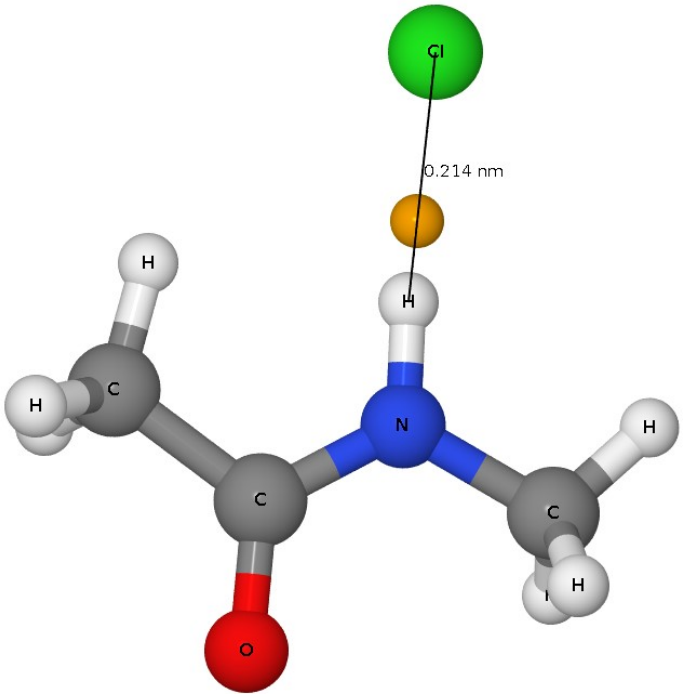

Figure S6: DFT gas phase $Cl(NMA)^-$ equilibrium geometry and critical point (3,-1) in orange**.**

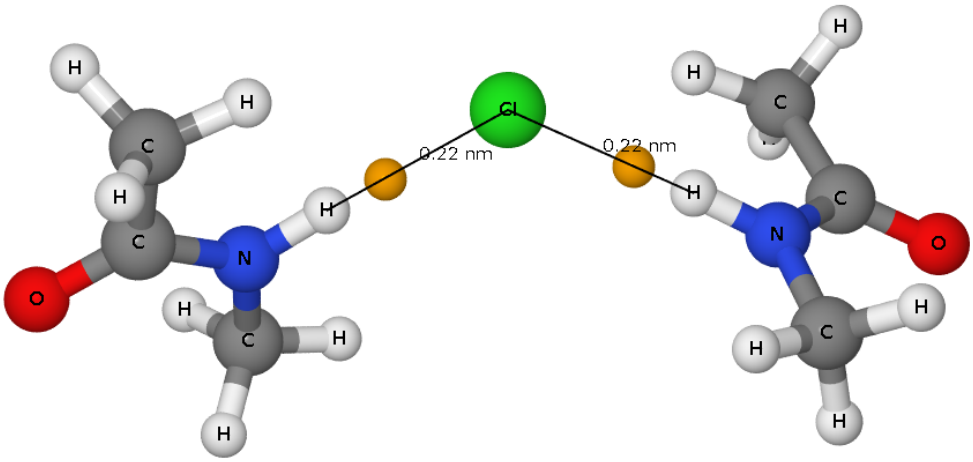

Figure S7: DFT gas phase $Cl(NMA)_2^-$ equilibrium geometry and critical point (3,-1) in orange**.**

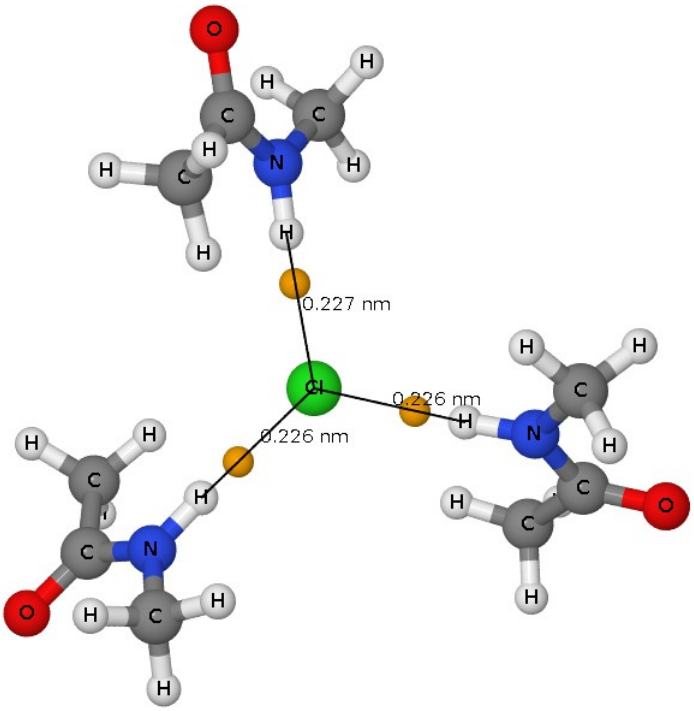

Figure S8: DFT gas phase $Cl(NMA)_3^-$ equilibrium geometry and critical point (3,-1) in orange**.**

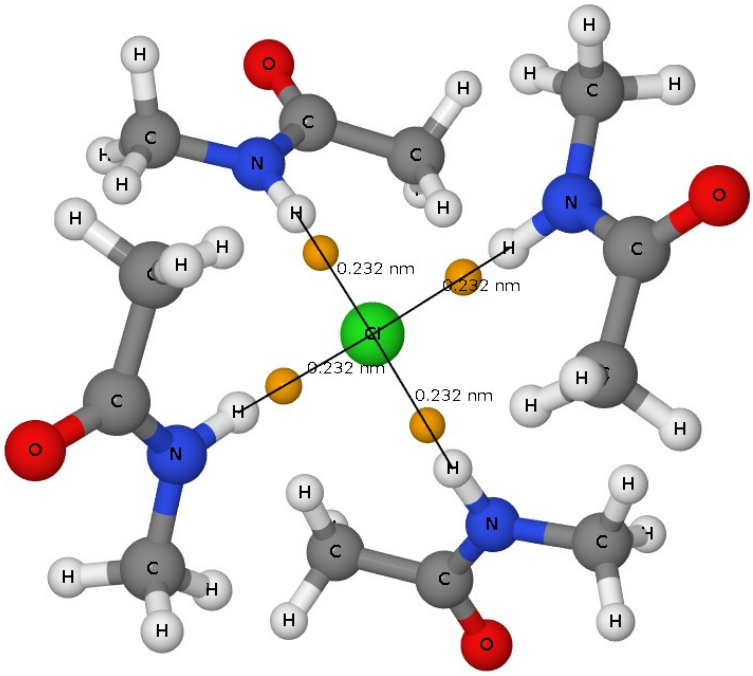

Figure S9: DFT gas phase $Cl(NMA)_4^-$ equilibrium geometry and critical point (3,-1) in orange**.**

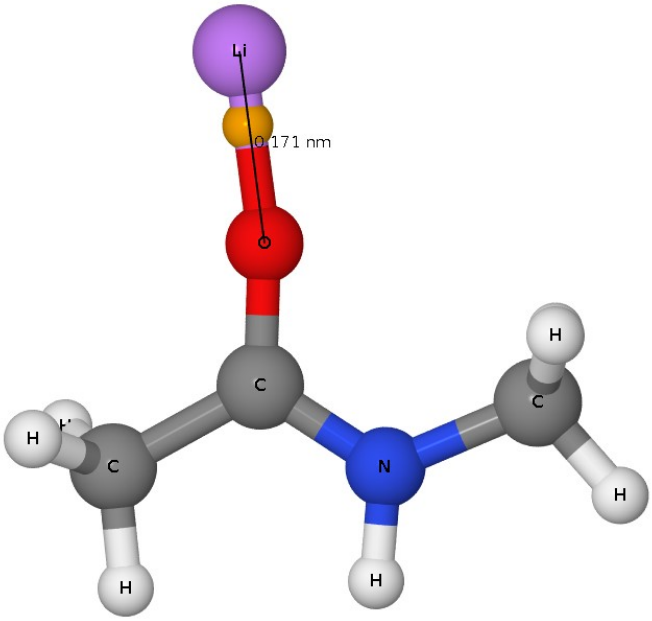

Figure S10: DFT gas phase $Li(NMA)_1^+$ equilibrium geometry and critical point (3,-1) in orange**.**

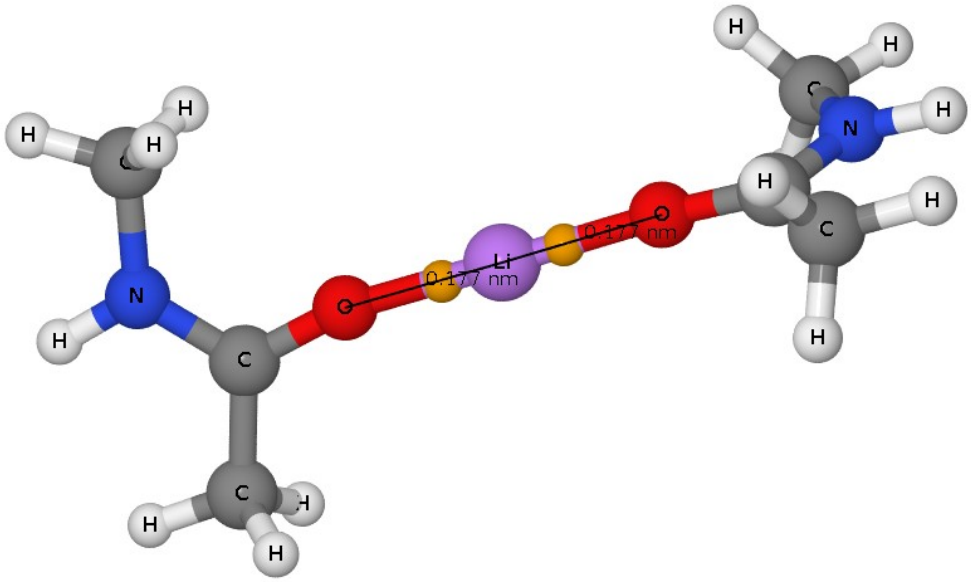

Figure S11: DFT gas phase $Li(NMA)_2^+$ equilibrium geometry and critical point (3,-1) in orange**.**

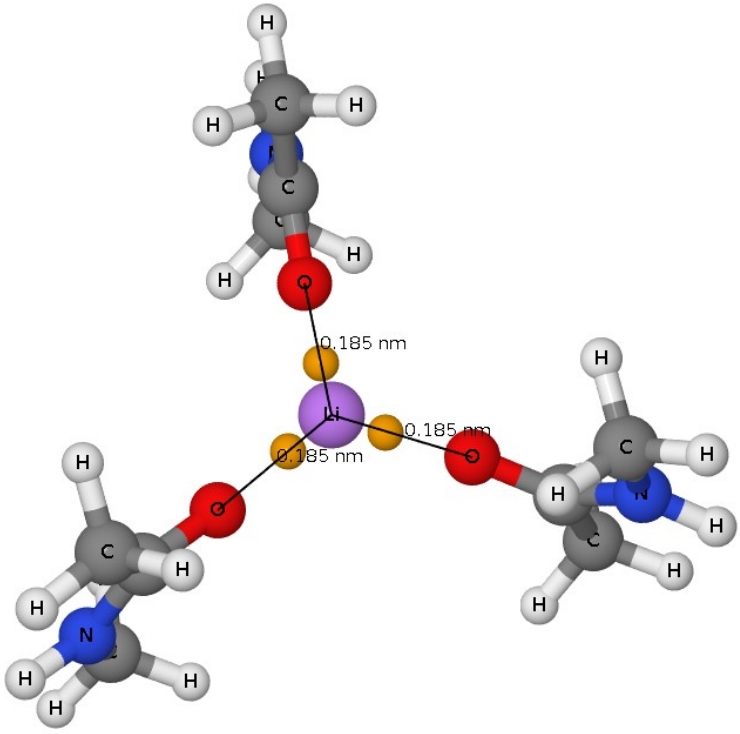

Figure S12: DFT gas phase $Li(NMA)_3^+$ equilibrium geometry and critical point (3,-1) in orange.

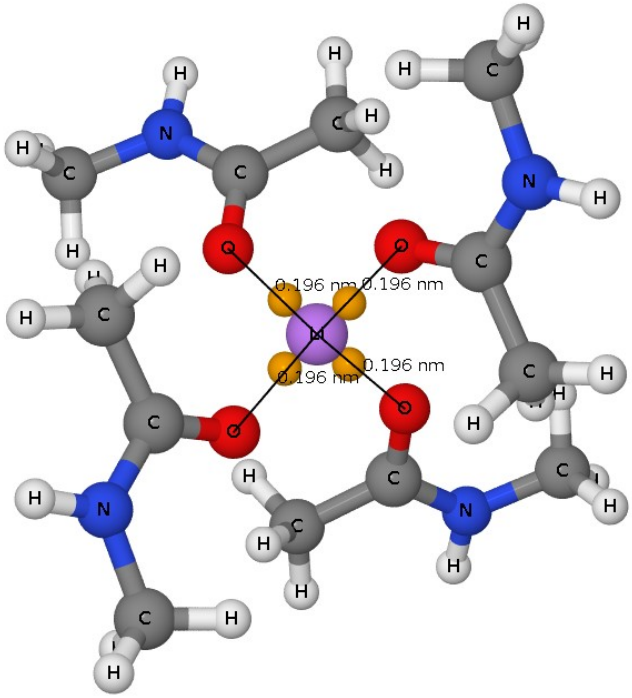

Figure S13: DFT gas phase $Li(NMA)_4^+$ equilibrium geometry and critical point (3,-1) in orange.

Table S5: Main chemical bond and bond angles averages for NMA molecule and $Cl(NMA)_x^-$ and $Li(NMA)_x^+$ complexes. Structural parameters obtained from the averages over all functionals. Bond distances are expressed in Angstrom and bond angles are in degree.

BOND	NMA	$Cl(NMA)_x^-$				$Li(NMA)_x^+$			
		1	2	3	4	1	2	3	4
CO	1.224	1.240	1.238	1.235	1.235	1.260	1.251	1.243	1.242
CN	1.412	1.397	1.399	1.401	1.404	1.397	1.400	1.402	1.404
CC	1.520	1.522	1.522	1.521	1.523	1.503	1.506	1.511	1.511
CH	1.095	1.097	1.097	1.096	1.096	1.094	1.094	1.094	1.095
NH	1.011	1.044	1.034	1.028	1.025	1.013	1.012	1.012	1.011
ClH	*Ø*	*2.105*	*2.172*	*2.233*	*2.292*	*Ø*	*Ø*	*Ø*	*Ø*
LiO	*Ø*	*Ø*	*Ø*	*Ø*	*Ø*	*1.724*	*1.783*	*1.861*	*1.962*

ANGLES	NMA	$Cl(NMA)_x^-$				$Li(NMA)_x^+$			
		1	2	3	4	1	2	3	4
OCC	121.8	121.7	121.8	121.9	121.8	120.8	121.2	121.5	121.6
OCN	122.9	123.5	123.2	123.0	122.9	120.6	120.8	121.4	121.6
CCN	115.3	114.8	115.0	115.1	115.3	118.6	118.0	117.1	116.9
CCH	110.4	109.9	110.0	110.0	110.1	110.4	110.4	110.4	110.2
CNH	118.6	a	119.3	119.3	119.3	118.1	118.4	118.4	118.3
HCH	108.8	108.9	108.8	108.8	108.8	108.8	108.8	108.8	108.9
CNC	122.7	a	121.5	121.5	121.4	123.9	123.3	123.2	123.3
HClH	*Ø*	*Ø*	*122.0*	*119.1*	*109.5*	*Ø*	*Ø*	*Ø*	*Ø*
OLiO	*Ø*	*Ø*	*Ø*	*Ø*	*Ø*	*Ø*	*179.3*	*120.0*	*109.5*

Table S6: Main chemical bonds distances and bonds angles of the NMA molecule. Bond distances are expressed in Angstrom and bond angles are in degree.

BOND	PBE	PW91	BLYP	TPSS	BMK	B3LYP	B3PW91	M06	μ	σ
CO	1.232	1.230	1.234	1.231	1.213	1.221	1.219	1.213	1.224	0.008
CN	1.414	1.413	1.424	1.417	1.406	1.411	1.405	1.404	1.412	0.007
CC	1.521	1.519	1.532	1.523	1.525	1.518	1.513	1.507	1.520	0.008
CH	1.100	1.099	1.099	1.095	1.093	1.092	1.092	1.093	1.095	0.003
NH	1.015	1.014	1.015	1.012	1.007	1.007	1.006	1.008	1.011	0.004
ANGLE	**PBE**	**PW91**	**BLYP**	**TPSS**	**BMK**	**B3LYP**	**B3PW91**	**M06**	**μ**	**σ**
OCC	122.0	122.0	121.9	122.0	121.5	121.7	121.7	121.8	121.8	0.2
OCN	122.7	122.8	122.9	122.7	123.0	122.9	122.9	123.1	122.9	0.1
CCN	115.2	115.3	115.3	115.3	115.5	115.4	115.4	115.2	115.3	0.1
CCH	110.5	110.4	110.4	110.3	110.1	110.4	110.4	110.4	110.4	0.1
CNH	118.7	118.7	118.4	118.7	118.7	118.5	118.6	118.8	118.6	0.1
HCH	108.7	108.7	108.8	109.0	108.9	108.7	108.7	108.6	108.8	0.1
CNC	122.7	122.6	123.1	122.6	122.7	123.0	122.8	122.5	122.7	0.2

Table S7: Main chemical bond distances, mean (μ) and standard deviation (σ) of the chemical bonds on different functionals of the $Cl(NMA)_x^-$ complexes. Values are expressed in Angstrom.

$Cl(NMA)_1^-$										
BOND	**PBE**	**PW91**	**BLYP**	**TPSS**	**BMK**	**B3LYP**	**B3PW91**	**M06**	**μ**	**σ**
CO	1.248	1.247	1.251	1.248	1.228	1.237	1.235	1.229	1.240	0.009
CN	1.400	1.399	1.409	1.402	1.392	1.396	1.391	1.389	1.397	0.007
CC	1.524	1.523	1.534	1.526	1.526	1.521	1.515	1.509	1.522	0.008
CH	1.102	1.100	1.100	1.097	1.095	1.093	1.094	1.095	1.097	0.003
NH	1.055	1.054	1.049	1.049	1.031	1.037	1.040	1.036	1.044	0.009
ClH	*2.063*	*2.058*	*2.133*	*2.087*	*2.147*	*2.136*	*2.099*	*2.115*	*2.105*	*0.034*

$Cl(NMA)_2^-$										
BOND	**PBE**	**PW91**	**BLYP**	**TPSS**	**BMK**	**B3LYP**	**B3PW91**	**M06**	**μ**	**σ**
CO	1.245	1.244	1.248	1.245	1.226	1.235	1.232	1.226	1.238	0.009
CN	1.402	1.401	1.411	1.405	1.394	1.398	1.393	1.391	1.399	0.007
CC	1.523	1.522	1.534	1.525	1.526	1.521	1.515	1.509	1.522	0.008
CH	1.101	1.100	1.100	1.096	1.094	1.093	1.094	1.095	1.097	0.003
NH	1.043	1.042	1.039	1.038	1.025	1.028	1.030	1.029	1.034	0.007
ClH	*2.138*	*2.131*	*2.208*	*2.158*	*2.201*	*2.203*	*2.172*	*2.169*	*2.172*	*0.030*

$Cl(NMA)_3^-$										
BOND	**PBE**	**PW91**	**BLYP**	**TPSS**	**BMK**	**B3LYP**	**B3PW91**	**M06**	**μ**	**σ**
CO	1.243	1.242	1.246	1.242	1.224	1.232	1.230	1.224	1.235	0.009
CN	1.404	1.403	1.413	1.407	1.396	1.400	1.395	1.393	1.401	0.007
CC	1.523	1.522	1.533	1.525	1.526	1.520	1.515	1.508	1.521	0.007
CH	1.101	1.099	1.099	1.096	1.094	1.093	1.093	1.094	1.096	0.003
NH	1.035	1.035	1.033	1.032	1.020	1.023	1.024	1.024	1.028	0.006
ClH	*2.202*	*2.192*	*2.272*	*2.220*	*2.270*	*2.262*	*2.235*	*2.213*	*2.233*	*0.031*

$Cl(NMA)_4^-$										
BOND	**PBE**	**PW91**	**BLYP**	**TPSS**	**BMK**	**B3LYP**	**B3PW91**	**M06**	**μ**	**σ**
CO	1.241	1.240	1.244	1.240	1.222	1.231	1.228	[a]	1.235	0.008
CN	1.406	1.405	1.415	1.409	1.397	1.402	1.397	[a]	1.404	0.006
CC	1.523	1.522	1.533	1.525	1.525	1.520	1.515	[a]	1.523	0.006
CH	1.101	1.099	1.099	1.096	1.094	1.092	1.093	[a]	1.096	0.003
NH	1.031	1.030	1.029	1.028	1.018	1.020	1.020	[a]	1.025	0.006
ClH	*2.253*	*2.244*	*2.336*	*2.283*	*2.313*	*2.318*	*2.295*	[a]	*2.292*	*0.034*

Table S8: Main chemical bond distances, mean (μ) and standard deviation (σ) of the chemical bonds on different functionals of the $Li(NMA)_x^+$ complexes. Values are expressed in Angstrom.

$Li(NMA)_1^+$										
BOND	**PBE**	**PW91**	**BLYP**	**TPSS**	**BMK**	**B3LYP**	**B3PW91**	**M06**	**μ**	**σ**
CO	1.267	1.266	1.272	1.267	1.249	1.259	1.255	1.249	1.260	0.009
CN	1.400	1.399	1.409	1.403	1.390	1.396	1.391	1.390	1.397	0.007
CC	1.503	1.502	1.513	1.507	1.508	1.502	1.497	1.490	1.503	0.007
CH	1.099	1.097	1.097	1.094	1.093	1.091	1.091	1.092	1.094	0.003
NH	1.017	1.016	1.017	1.014	1.010	1.010	1.009	1.011	1.013	0.004
LiO	*1.726*	*1.725*	*1.725*	*1.724*	*1.724*	*1.714*	*1.724*	*1.729*	*1.724*	*0.004*

$Li(NMA)_2^+$										
BOND	**PBE**	**PW91**	**BLYP**	**TPSS**	**BMK**	**B3LYP**	**B3PW91**	**M06**	**μ**	**σ**
CO	1.258	1.257	1.262	1.258	1.240	1.249	1.246	1.240	1.251	0.009
CN	1.402	1.401	1.411	1.405	1.393	1.398	1.393	1.392	1.400	0.007
CC	1.506	1.505	1.517	1.510	1.512	1.506	1.501	1.494	1.506	0.007
CH	1.099	1.097	1.097	1.094	1.093	1.091	1.091	1.092	1.094	0.003
NH	1.016	1.015	1.016	1.013	1.009	1.009	1.008	1.010	1.012	0.004
LiO	*1.784*	*1.783*	*1.786*	*1.782*	*1.778*	*1.772*	*1.783*	*1.799*	*1.783*	*0.008*

$Li(NMA)_3^+$										
BOND	**PBE**	**PW91**	**BLYP**	**TPSS**	**BMK**	**B3LYP**	**B3PW91**	**M06**	**μ**	**σ**
CO	1.250	1.249	1.253	1.249	1.231	1.240	1.237	1.231	1.243	0.009
CN	1.405	1.404	1.414	1.408	1.396	1.401	1.396	1.395	1.402	0.007
CC	1.511	1.510	1.522	1.515	1.515	1.510	1.505	1.497	1.511	0.007
CH	1.099	1.097	1.098	1.094	1.093	1.091	1.092	1.092	1.094	0.003
NH	1.016	1.015	1.016	1.013	1.008	1.008	1.007	1.009	1.012	0.004
LiO	*1.867*	*1.868*	*1.869*	*1.868*	*1.834*	*1.851*	*1.865*	*1.867*	*1.861*	*0.012*

$Li(NMA)_4^+$										
BOND	**PBE**	**PW91**	**BLYP**	**TPSS**	**BMK**	**B3LYP**	**B3PW91**	**M06**	**μ**	**σ**
CO	1.249	1.248	1.251	1.248	1.233	1.239	1.236	1.233	1.242	0.008
CN	1.407	1.406	1.416	1.410	1.397	1.403	1.398	1.396	1.404	0.007
CC	1.512	1.511	1.523	1.516	1.515	1.511	1.506	1.498	1.511	0.008
CH	1.100	1.098	1.098	1.094	1.093	1.091	1.092	1.093	1.095	0.003
NH	1.016	1.015	1.016	1.013	1.008	1.008	1.007	1.008	1.011	0.004
LiO	*1.971*	*1.969*	*1.983*	*1.974*	*1.924*	*1.959*	*1.971*	*1.947*	*1.962*	*0.019*

Table S9 Main chemical bond angles, mean (μ) and standard deviation (σ) of the chemical bond angles on different functionals of the $Cl(NMA)_x^-$ complexes. Values are expressed in degrees.

$Cl(NMA)_1^-$										
ANGLE	**PBE**	**PW91**	**BLYP**	**TPSS**	**BMK**	**B3LYP**	**B3PW91**	**M06**	**μ**	**σ**
OCC	121.8	121.9	121.5	121.9	121.6	121.5	121.7	121.8	121.7	0.2
OCN	123.6	123.5	123.6	123.4	123.4	123.5	123.5	123.7	123.5	0.1
CCN	114.6	114.6	114.9	114.7	115.0	115.1	114.9	114.6	114.8	0.2
CCH	109.9	109.9	110.0	109.8	109.6	109.9	109.9	110.0	109.9	0.1
CNH	[a]	[a]	[a]	[a]	[a]	[a]	[a]	[a]		
HCH	108.8	108.8	108.8	109.0	109.1	108.8	108.8	108.7	108.9	0.1
CNC	[a]	[a]	[a]	[a]	[a]	[a]	[a]	[a]		
HClH	***ø***	***ø***	***ø***	***ø***	***ø***	***ø***	***ø***	***ø***	***ø***	***ø***

$Cl(NMA)_2^-$										
ANGLE	**PBE**	**PW91**	**BLYP**	**TPSS**	**BMK**	**B3LYP**	**B3PW91**	**M06**	**μ**	**σ**
OCC	122.0	121.9	121.7	122.0	121.7	121.6	121.8	121.8	121.8	0.1
OCN	123.2	123.2	123.3	123.1	123.2	123.2	123.2	123.4	123.2	0.1
CCN	114.8	114.8	115.1	114.9	115.1	115.2	115.1	114.8	115.0	0.2
CCH	110.0	110.0	110.1	109.9	109.7	110.0	110.0	110.1	110.0	0.1
CNH	119.3	119.3	119.1	119.4	119.3	119.2	119.3	119.3	119.3	0.1
HCH	108.8	108.8	108.8	109.0	109.0	108.8	108.8	108.7	108.8	0.1
CNC	121.4	121.4	121.8	121.3	121.4	121.6	121.4	121.5	121.5	0.2
HClH	*115.8*	*112.4*	*123.7*	*118.8*	*a*	*124.6*	*121.9*	*137.2*	*122.0*	*8.0*

$Cl(NMA)_3^-$										
ANGLE	**PBE**	**PW91**	**BLYP**	**TPSS**	**BMK**	**B3LYP**	**B3PW91**	**M06**	**μ**	**σ**
OCC	122.0	122.0	121.7	122.1	121.8	121.7	121.8	121.9	121.9	0.2
OCN	123.0	123.0	123.0	122.8	123.0	123.0	123.0	123.2	123.0	0.1
CCN	115.0	115.0	115.2	115.1	115.2	115.3	115.2	114.9	115.1	0.2
CCH	110.1	110.1	110.1	109.9	109.7	110.0	110.0	110.1	110.0	0.1
CNH	119.3	119.3	119.1	119.3	119.3	119.2	119.3	119.3	119.3	0.1
HCH	108.7	108.7	108.8	109.0	109.0	108.8	108.8	108.6	108.8	0.1
CNC	121.5	121.4	121.8	121.3	121.3	121.6	121.4	121.4	121.5	0.2
HClH	*118.8*	*118.1*	*119.5*	*119.0*	*118.8*	*119.4*	*119.2*	*119.9*	*119.1*	*0.5*

$Cl(NMA)_4^-$										
ANGLE	**PBE**	**PW91**	**BLYP**	**TPSS**	**BMK**	**B3LYP**	**B3PW91**	**M06**	**μ**	**σ**
OCC	122.0	122.0	121.7	121.8	121.8	121.6	121.8	[a]	121.8	0.1
OCN	122.8	122.8	122.8	123.3	122.8	122.8	122.8	[a]	122.9	0.2
CCN	115.2	115.2	115.5	114.9	115.4	115.6	115.4	[a]	115.3	0.2
CCH	110.2	110.2	110.2	110.0	109.8	110.1	110.1	[a]	110.1	0.1
CNH	119.3	119.3	119.2	119.1	119.4	119.3	119.4	[a]	119.3	0.1
HCH	108.7	108.7	108.7	109.0	109.0	108.7	108.7	[a]	108.8	0.1
CNC	121.4	121.3	121.6	121.9	121.2	121.5	121.3	[a]	121.4	0.2
HClH	*109.5*	*109.4*	*109.5*	*109.6*	*109.5*	*109.5*	*109.5*	*[a]*	*109.5*	*0.1*

Table S10 Main chemical bond angles, mean (μ) and standard deviation (σ) of the chemical bond angles on different functionals of the $Li(NMA)_x^+$ complexes. Values are expressed in degrees.

$Li(NMA)_1^+$										
ANGLE	**PBE**	**PW91**	**BLYP**	**TPSS**	**BMK**	**B3LYP**	**B3PW91**	**M06**	**μ**	**σ**
OCC	121.0	121.0	120.8	121.0	120.6	120.6	120.8	120.7	120.8	0.2
OCN	120.4	120.4	120.6	120.3	120.8	120.7	120.6	120.8	120.6	0.2
CCN	118.6	118.6	118.7	118.7	118.7	118.7	118.6	118.5	118.6	0.1
CCH	110.5	110.5	110.5	110.3	110.1	110.4	110.4	110.5	110.4	0.1
CNH	118.0	118.1	117.8	118.1	118.2	118.0	118.1	118.3	118.1	0.2
HCH	108.7	108.7	108.8	109.1	109.0	108.8	108.8	108.6	108.8	0.1
CNC	123.9	123.9	124.4	123.9	123.5	124.1	123.9	123.3	123.9	0.3
OLiO	*Ø*	*Ø*	*Ø*	*Ø*	*Ø*	*Ø*	*Ø*	*Ø*	*Ø*	*Ø*

$Li(NMA)_2^+$										
ANGLE	**PBE**	**PW91**	**BLYP**	**TPSS**	**BMK**	**B3LYP**	**B3PW91**	**M06**	**μ**	**σ**
OCC	121.4	121.4	121.2	121.4	121.0	121.0	121.1	121.1	121.2	0.2
OCN	120.7	120.6	120.8	120.5	121.0	120.9	120.9	121.1	120.8	0.2
CCN	118.0	118.0	118.0	118.1	118.1	118.1	118.0	117.9	118.0	0.1
CCH	110.5	110.5	110.5	110.3	110.1	110.4	110.4	110.5	110.4	0.1
CNH	118.3	118.4	118.1	118.4	118.5	118.3	118.3	118.6	118.4	0.2
HCH	108.7	108.7	108.8	109.0	108.9	108.8	108.7	108.6	108.8	0.1
CNC	123.3	123.3	123.8	123.3	122.9	123.5	123.3	122.7	123.3	0.3
OLiO	*179.3*	*179.2*	*179.2*	*179.1*	*179.8*	*179.5*	*179.5*	*178.8*	*179.3*	*0.3*

$Li(NMA)_3^+$										
ANGLE	**PBE**	**PW91**	**BLYP**	**TPSS**	**BMK**	**B3LYP**	**B3PW91**	**M06**	**μ**	**σ**
OCC	121.4	121.4	121.6	121.4	121.3	121.4	121.6	121.4	121.5	0.1
OCN	121.9	121.8	121.1	121.8	121.2	121.2	121.1	121.3	121.4	0.3
CCN	116.7	116.8	117.3	116.8	117.5	117.4	117.3	117.2	117.1	0.3
CCH	110.5	110.5	110.5	110.3	110.1	110.4	110.4	110.5	110.4	0.1
CNH	117.9	118.0	118.4	117.9	118.8	118.5	118.6	118.9	118.4	0.4
HCH	108.8	108.8	108.7	109.1	108.9	108.8	108.7	108.6	108.8	0.2
CNC	124.2	124.1	123.2	124.1	122.4	122.9	122.8	122.2	123.2	0.8
OLiO	*119.99*	*120.00*	*120.00*	*119.99*	*120.00*	*120.00*	*120.00*	*120.00*	*120.0*	*0.0*

$Li(NMA)_4^+$										
ANGLE	**PBE**	**PW91**	**BLYP**	**TPSS**	**BMK**	**B3LYP**	**B3PW91**	**M06**	**μ**	**σ**
OCC	121.6	121.6	121.7	121.8	121.2	121.6	121.6	121.5	121.6	0.2
OCN	121.8	121.7	121.6	121.7	121.2	121.5	121.8	121.1	121.6	0.3
CCN	116.6	116.7	116.6	116.6	117.6	116.9	116.6	117.4	116.9	0.4
CCH	110.3	110.3	110.3	110.1	109.8	110.2	110.2	110.2	110.2	0.2
CNH	118.1	118.1	118.0	118.1	118.7	118.3	118.1	119.0	118.3	0.4
HCH	108.8	108.8	108.9	109.1	109.0	108.8	108.8	108.7	108.9	0.1
CNC	123.9	123.7	123.9	123.7	122.5	123.3	123.7	122.0	123.3	0.7
OLiO	*109.5*	*109.5*	*109.5*	*109.5*	*109.5*	*109.5*	*109.5*	*109.5*	*109.5*	*0.0*

Table S11: Interaction energies ($\Delta_R E$) of $Li(NMA)^+$ and $Cl(NMA)^-$ complexes calculated on different force-fields (C27/NBFIX1, C27/NBFIX2, Cheatham, Drude) and on PBE/Def2-TZVPD . All values are expressed in kcal/mol.

Ion	(NMA)x	PBE		B3LYP		Force Fields			
		Def2-TZVPD	6-311+(d,p)	Def2-TZVPD	6-311+(d,p)	C27/NBFIX1	C27/NBFIX2	Cheatham	Drude
Cl^-	1	-23.1	-22.7	-21.1	-20.7	-17.9	-17.9	-16.7	-24.1
	2	-41.1	-40.4	-37.8	-37.3	-35.7	-35.7	-33.5	-44.6
Li^+	1	-55.9	-55.6	-57.9	-57.5	-38.9	-46.4	-39.5	-56.9
	2	-96.5	-96.2	-99.8	-99.5	-74.1	-92.3	-78.9	-96.8

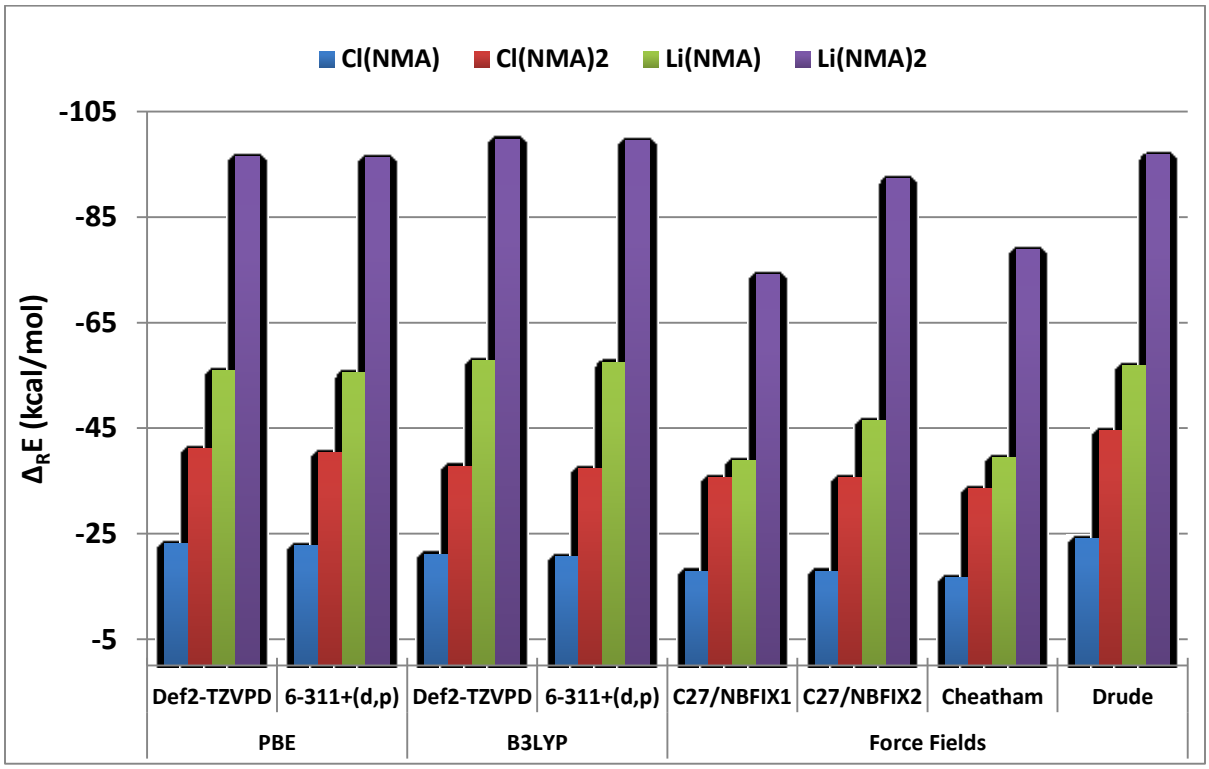

Figure S14: Electronic binding energies ($\Delta_R E$) calculated at LiCl(NMA) and $LiCl(NMA)_2$ complexes on different methods and level of theory.

Table S12: Chemical bond and angle bond values of of $Li(NMA)^+$ and $Cl(NMA)^-$ complexes calculated on different force-fields (C27/NBFIX1, C27/NBFIX2, Cheatham, Drude) and on PBE/Def2-TZVPD . Chemical bond lengths are expressed in Å and angle bonds in degrees.

Ion	$(NMA)_x$	Bond	PBE		B3LYP		Force Fields			
			Def2-TZVPD	6-311+(d,p)	Def2-TZVPD	6-311+(d,p)	C27/NBFIX1	C27/NBFIX2	Cheatham	Drude
Li^+	1	O_1-Li^+	1.716	1.726	1.704	1.714	1.905	1.63	1.845	1.88
	2	O_2-Li^+	1.779	1.784	1.767	1.772	1.92	1.67	1.845	1.92
Cl^-	1	H_1-Cl^-	2.056	2.063	2.132	2.136	2.2	2.2	2.23	2.11
	2	H_2-Cl^-	2.134	2.138	2.201	2.203	2.21	2.21	2.25	2.17

Ion	(NMA)x	Angle	PBE		B3LYP		Force Fields			
			Def2-TZVPD	6-311+(d,p)	Def2-TZVPD	6-311+(d,p)	C27/NBFIX1	C27/NBFIX2	Cheatham	Drude
Li^+	2	O-Li^+-O	179.1	179.3	179.4	179.5	112.7	176.5	176.8	175.9
Cl^-	2	H-Cl^--H	111.1	115.8	122.7	124.6	72.04	72.04	71.7	69.4

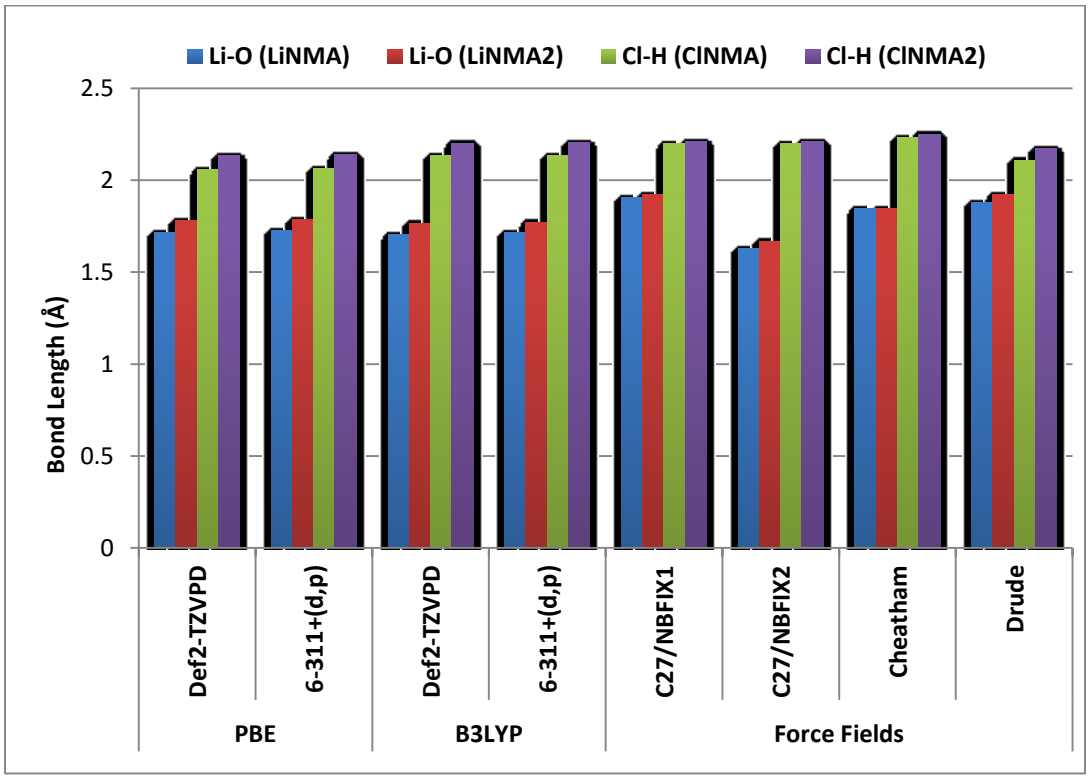

Figure S15: Bond lengths for Li^+-O and Cl^--H at LiCl(NMA) and $LiCl(NMA)_2$ complexes on different methods and level of theory.

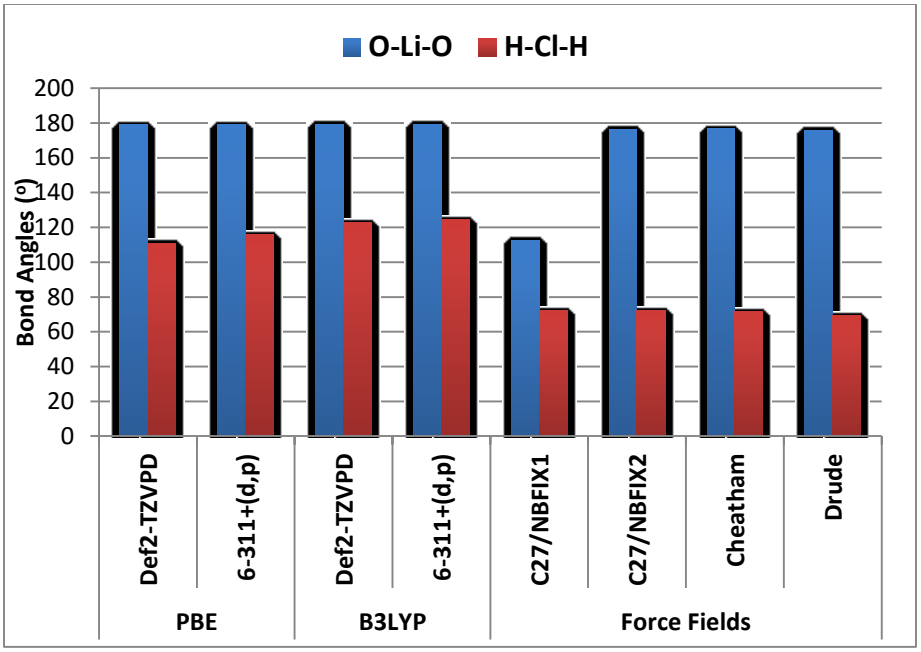

Figure S16: Bond angles for O-Li^+-O and H-Cl^- - H at $LiCl(NMA)_2$ complex on different methods and level of theory.

Table S13 Thermodynamic functions of $Li(NMA)_x^+$ and $Cl(NMA)_x^-$ complex formation for PBE, TPSS and B3LYP functional with 6-311+G(d,p) (B_0) and Def2-TZVPD (B_1) basis set and their differences (ΔF). All values are expressed in kcal.mol^{-1} and θ refers to 1 mol, 298.15 K and 1 bar standard conditions.

$\Delta_R E$

A(NMA)$_n$		B_1 = Def2-TZVPD			B_0 = 6-311+G(d,p)			$\Delta F(B_1-B_0)$		
A	**n**	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**
Cl^-	**1**	-23.1	-21.7	-21.1	-22.7	-21.4	-20.7	-0.4	-0.3	-0.3
	2	-41.1	-38.7	-37.8	-40.4	-38.2	-37.3	-0.7	-0.5	-0.5
Li^+	**1**	-55.9	-56.1	-57.9	-55.6	-55.8	-57.5	-0.4	-0.3	-0.3
	1	-96.5	-96.7	-99.8	-96.2	-96.4	-99.5	-0.4	-0.3	-0.3

$\Delta_R H^\theta$

A(NMA)$_n$		B_1 = Def2-TZVPD			B_0 = 6-311+G(d,p)			$\Delta F(B_1-B_0)$		
A	**n**	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**
Cl^-	**1**	-23.3	-21.9	-21.0	-22.9	-21.5	-20.6	-0.4	-0.3	-0.4
	2	-40.1	-38.2	-36.5	-39.4	-37.1	-35.9	-0.8	-1.1	-0.5
Li^+	**1**	-54.7	-54.8	-56.6	-54.3	-55.1	-56.3	-0.4	0.3	-0.3
	2	-93.4	-93.6	-96.7	-93.1	-93.3	-96.4	-0.3	-0.3	-0.2

$\Delta_R G^\theta$

A(NMA)$_n$		B_1 = Def2-TZVPD			B_0 = 6-311+G(d,p)			$\Delta F(B_1-B_0)$		
A	**n**	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**
Cl^-	**1**	-16.5	-15.2	-13.6	-15.9	-14.5	-13.0	-0.6	-0.6	-0.6
	2	-27.0	-23.0	-22.5	-25.7	-23.0	-20.8	-1.3	0.0	-1.7
Li^+	**1**	-47.5	-47.8	-48.5	-47.1	-46.1	-48.0	-0.4	-1.8	-0.5
	2	-77.9	-78.2	-79.9	-77.3	-77.5	-78.9	-0.6	-0.7	-1.0

$-T\Delta_R S^\theta$

A(NMA)$_n$		B_1 = Def2-TZVPD			B_0 = 6-311+G(d,p)			$\Delta F(B_1-B_0)$		
A	**n**	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**
Cl^-	**1**	6.9	6.7	7.4	7.0	7.0	7.6	-0.1	0.3	0.3
	2	13.1	15.2	14.0	13.7	14.1	15.2	-0.6	-1.1	1.2
Li^+	**1**	7.2	7.0	8.1	7.2	9.0	8.3	0.0	2.0	0.2
	2	15.5	15.3	16.8	15.8	15.7	17.5	-0.3	0.4	0.7

Table S14: Main distance and angle bonds characterized to $Cl(NMA)^-$ and $Cl(NMA)_2^-$ in the PBE, TPSS and B3LYP functional using the basis sets Def2-TZVPD(B1) and 6-311+G(d,p)(B0) and their differences (ΔF). Bonds distances are expressed in Å and bond angles are in degrees.

$Cl(NMA)^-$

	B_1 = Def2-TZVPD			B_0 = 6-311+G(d,p)			ΔF(B_1-B_0)		
Bonds	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**
CO	1.246	1.245	1.236	1.248	1.248	1.237	-0.002	-0.002	-0.002
CN	1.396	1.399	1.393	1.400	1.402	1.396	-0.003	-0.004	-0.004
CC	1.521	1.523	1.518	1.524	1.526	1.521	-0.002	-0.002	-0.002
CH	1.101	1.096	1.092	1.102	1.097	1.093	-0.001	-0.001	-0.001
NH	1.055	1.048	1.036	1.055	1.049	1.037	0.000	-0.001	-0.001
HCl	2.056	2.086	2.132	2.063	2.087	2.136	-0.007	-0.001	-0.004
Angles	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**
OCC	121.8	121.9	121.4	121.8	121.9	121.5	-0.05	-0.04	-0.08
OCN	123.6	123.4	123.5	123.6	123.4	123.5	0.03	0.02	0.00
CCN	114.6	114.8	115.1	114.6	114.7	115.1	0.03	0.03	0.08
CCH_c	109.9	109.8	109.9	109.9	109.8	109.9	-0.03	0.01	0.01
HCH	108.8	109.0	108.8	108.8	109.0	108.8	-0.02	-0.05	-0.04

$Cl(NMA)_2^-$

	B_1 = Def2-TZVPD			B_0 = 6-311+G(d,p)			ΔF(B_1-B_0)		
Bonds	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**
CO	1.243	1.242	1.233	1.245	1.245	1.235	-0.002	-0.002	-0.002
CN	1.399	1.401	1.395	1.402	1.405	1.398	-0.003	-0.004	-0.004
CC	1.521	1.523	1.518	1.523	1.525	1.521	-0.002	-0.003	-0.003
CH	1.100	1.095	1.092	1.101	1.096	1.093	-0.001	-0.001	-0.001
NH	1.042	1.038	1.027	1.043	1.038	1.028	0.000	-0.001	-0.001
HCl	2.134	2.158	2.201	2.138	2.158	2.203	-0.004	0.000	-0.002
Angles	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**
OCC	121.9	121.9	121.5	122.0	122.0	121.6	-0.08	-0.06	-0.11
OCN	123.2	123.1	123.2	123.2	123.1	123.2	0.00	0.00	-0.01
CCN	114.9	115.0	115.3	114.8	114.9	115.2	0.07	0.07	0.12
CCH_c	110.0	109.9	110.0	110.0	109.9	110.0	-0.01	0.02	0.01
HCH	108.7	108.9	108.8	108.8	109.0	108.8	-0.03	-0.05	-0.04
CNH	119.3	119.4	119.2	119.3	119.4	119.2	-0.02	-0.02	-0.02
CNC	121.4	121.3	121.7	121.4	121.3	121.6	0.03	0.03	0.03
HClH	111.1	113.9	122.7	115.8	118.8	124.6	-4.70	-4.86	-1.84

Table S15: Main distance and angle bonds characterized to $Li(NMA)^+$ and $Li(NMA)_2^+$ in the PBE, TPSS and B3LYP functional using the basis sets Def2-TZVPD(B1) and 6-311+G(d,p)(B0) and their differences (ΔF). Bonds distances are expressed in Å and bond angles are in degrees.

$Li(NMA)^+$

	B_1 = Def2-TZVPD			B_0 = 6-311+G(d,p)			$\Delta F(B_1-B_0)$		
Bonds	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**
CO	1.264	1.264	1.256	1.267	1.267	1.259	-0.002	-0.003	-0.003
CN	1.396	1.399	1.392	1.400	1.403	1.396	-0.003	-0.004	-0.004
CC	1.501	1.504	1.500	1.503	1.507	1.502	-0.002	-0.002	-0.002
CH	1.098	1.093	1.090	1.099	1.094	1.091	-0.001	-0.001	-0.001
NH	1.016	1.013	1.008	1.017	1.014	1.010	-0.001	-0.001	-0.002
OLi	1.716	1.712	1.704	1.726	1.724	1.714	-0.010	-0.012	-0.010
Angles	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**
OCC	121.0	121.0	120.6	121.0	121.0	120.6	0.01	0.01	0.00
OCN	120.5	120.4	120.7	120.4	120.3	120.7	0.08	0.11	0.05
CCN	118.5	118.6	118.7	118.6	118.7	118.7	-0.09	-0.12	-0.06
CCH_c	110.5	110.3	110.4	110.5	110.3	110.4	-0.04	0.00	-0.02
HCH	108.7	109.0	108.8	108.7	109.1	108.8	0.00	-0.03	-0.02
CNH	118.0	118.0	117.9	118.0	118.1	118.0	-0.05	-0.06	-0.05
CNC	124.0	124.0	124.2	123.9	123.9	124.1	0.10	0.12	0.10

$Li(NMA)_2^+$

	B_1 = Def2-TZVPD			B_0 = 6-311+G(d,p)			$\Delta F(B_1-B_0)$		
Bonds	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**
CO	1.256	1.255	1.247	1.258	1.258	1.249	-0.002	-0.003	-0.002
CN	1.399	1.401	1.395	1.402	1.405	1.398	-0.004	-0.004	-0.004
CC	1.504	1.508	1.503	1.506	1.510	1.506	-0.002	-0.002	-0.002
CH	1.098	1.093	1.090	1.099	1.094	1.091	-0.001	-0.001	-0.001
NH	1.015	1.012	1.007	1.016	1.013	1.009	-0.001	-0.001	-0.002
OLi	1.779	1.776	1.767	1.784	1.782	1.772	-0.005	-0.006	-0.005
Angles	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**	**PBE**	**TPSS**	**B3LYP**
OCC	121.4	121.4	121.0	121.4	121.4	121.0	0.00	0.00	-0.02
OCN	120.7	120.6	120.9	120.7	120.5	120.9	0.06	0.08	0.05
CCN	117.9	118.0	118.1	118.0	118.1	118.1	-0.06	-0.08	-0.03
CCH_c	110.5	110.3	110.4	110.5	110.3	110.4	-0.04	0.00	-0.02
HCH	108.7	109.0	110.4	108.7	109.0	108.8	-0.01	-0.04	1.56
CNH	118.3	118.3	118.2	118.3	118.4	118.3	-0.04	-0.06	-0.06
CNC	123.4	123.4	123.6	123.3	123.3	123.5	0.09	0.12	0.11
OLiO	179.1	179.0	179.4	179.3	179.1	179.5	-0.17	-0.09	-0.09

III. QTAIM critical point analysis.

Using the Quantum Theory of Atoms in Molecules (QTAIM) proposed by Bader the saddle (3,-1) critical points (CP) type were characterized between all pairs of atoms, but only those between Cl-H and Li-O will be presented and discussed here. These critical points describe the chemical interactions between the ions (Li^+ and Cl^-) and the NMA molecules. The CP(3,-1) localizations are presented on Figures S6 to S13 as orange dots. On those critical points the electronic density (ρ) and the electronic Laplacian ($\nabla^2\rho$) were calculated using the B3LYP/6-311+G** level of theory as well as the Hessian matrix eigenvalue (λ_i) and energetic components (H,K,V), Tables S16 and S17. The critical point analysis was done with MultiWFN and JMol softwares to provide the numerical values analysis and the visual representation of these properties presented on Figures S17 to S23. The electron localization functions (ELF) pictures were created to all complex and are also presented below.

An electronic density below 0.2 describes a weak interaction and a positive value of the Laplacian describes a closed-shell interaction. Then, considering the values presented in the Tables S16 and S17, there are a non-covalent bond interactions between the ions and the NMA molecules. The van der Waals (VDW) interactions are characterized with a very close zero density in the CP, in all the complexes the electronic density is small but they cannot be considered as VDW interactions. The CP analysis pointed that there are interaction between the ions and NMA molecules but they are of ionic predominant types. Values of $|\lambda 1|/\lambda 3 < 1$ also points out closed-shell interaction as well as $|V|/G < 1$ values indicate weak close-shell interaction. As the density in the CP are greater then 0.001, we can claim that there are H-bond interactions between Cl-H(NMA) bonds and there are ionic interactions on Li-O(NM) bonds. The ELF structures do not show any shared electrons between ions and NMA molecules and in the case of the $Li(NMA)_n^+$ complexes there is a strong polarization effect over the O atoms of the NMA molecule, Figures S24, S26 and S28. Polarization effects were also captured in the ELF structure of $Cl(NMA)_n^-$ complexes in principal over the Cl^- anion.

Table S16: The electronic density (ρ), the electronic density Laplacian ($\nabla^2\rho$), the electronic Hessian matrix eigenvalue (λ_i), electronic energy (H), electronic kinetic energy (K) and electronic potential energy (K) values for $Cl(NMA)_n^-$ complexes evaluated onto its critical point of type (3,-1) in B3LYP/6-311+G** level of theory.

#NMA	ρ	$\nabla^2\rho$	λ1	λ2	λ3	|λ1|/λ3	H	K	V	|V|/G
1	0.03019	0.06789	-0.03710	-0.03635	0.14135	0.26250	-0.001486	0.018459	-0.019945	1.080
2	0.02550	0.06472	-0.02924	-0.02990	0.12386	0.23607	0.000157	0.016023	-0.015865	0.990
	0.02533	0.06441	-0.02966	-0.02893	0.12301	0.24116	0.000214	0.015889	-0.015675	0.987
3	0.02223	0.06079	-0.02504	-0.02438	0.11021	0.22719	0.001025	0.014172	-0.013147	0.928
	0.02197	0.06042	-0.02467	-0.02400	0.10910	0.22616	0.001084	0.014022	-0.012938	0.923
	0.02184	0.06001	-0.02444	-0.02379	0.10824	0.22580	0.001107	0.013896	-0.012789	0.920
4	0.01952	0.05611	-0.02106	-0.02047	0.09764	0.21572	0.001527	0.012500	-0.010973	0.878
	0.01935	0.05564	-0.02079	-0.02020	0.09663	0.21517	0.001548	0.012363	-0.010815	0.875
	0.01950	0.05600	-0.02101	-0.02041	0.09742	0.21566	0.001529	0.012471	-0.010942	0.877
	0.01945	0.05588	-0.02093	-0.02034	0.09715	0.21548	0.001535	0.012436	-0.010901	0.877

Table S17: The electronic density (ρ), the electronic density Laplacian ($\nabla^2\rho$), the electronic Hessian matrix eigenvalue (λ_i), electronic energy (H), electronic kinetic energy (K) and electronic potential energy (K) values for $Li(NMA)_n^+$ complexes evaluated onto its critical point of type (3,-1) in B3LYP/6-311+G** level of theory.

#NMA	ρ(r)	Lap(r)	λ1	λ2	λ3	|λ1|/λ3	H	K	V	|V|/G
1	0.04738	0.42414	-0.09516	-0.09099	0.61029	0.15593	0.017945	0.088090	-0.070146	0.7963
2	0.04057	0.34032	-0.07915	-0.07584	0.49532	0.15979	0.014874	0.070207	-0.055333	0.7881
	0.04055	0.33997	-0.07909	-0.07581	0.49487	0.15981	0.014858	0.070135	-0.055277	0.7882
3	0.03192	0.25907	-0.05950	-0.05715	0.37571	0.15836	0.012483	0.052284	-0.039802	0.7613
	0.03193	0.25843	-0.05943	-0.05723	0.37509	0.15843	0.012433	0.052174	-0.039741	0.7617
	0.03191	0.25931	-0.05949	-0.05710	0.37590	0.15827	0.012505	0.052322	-0.039817	0.7610
4	0.02580	0.18705	-0.04449	-0.04389	0.27544	0.16153	0.008844	0.037919	-0.029075	0.7668
	0.02567	0.18621	-0.04421	-0.04362	0.27404	0.16132	0.008819	0.037733	-0.028914	0.7663
	0.02580	0.18805	-0.04452	-0.04402	0.27659	0.16096	0.008930	0.038083	-0.029152	0.7655
	0.02592	0.18865	-0.04476	-0.04426	0.27767	0.16121	0.008940	0.038223	-0.029283	0.7661

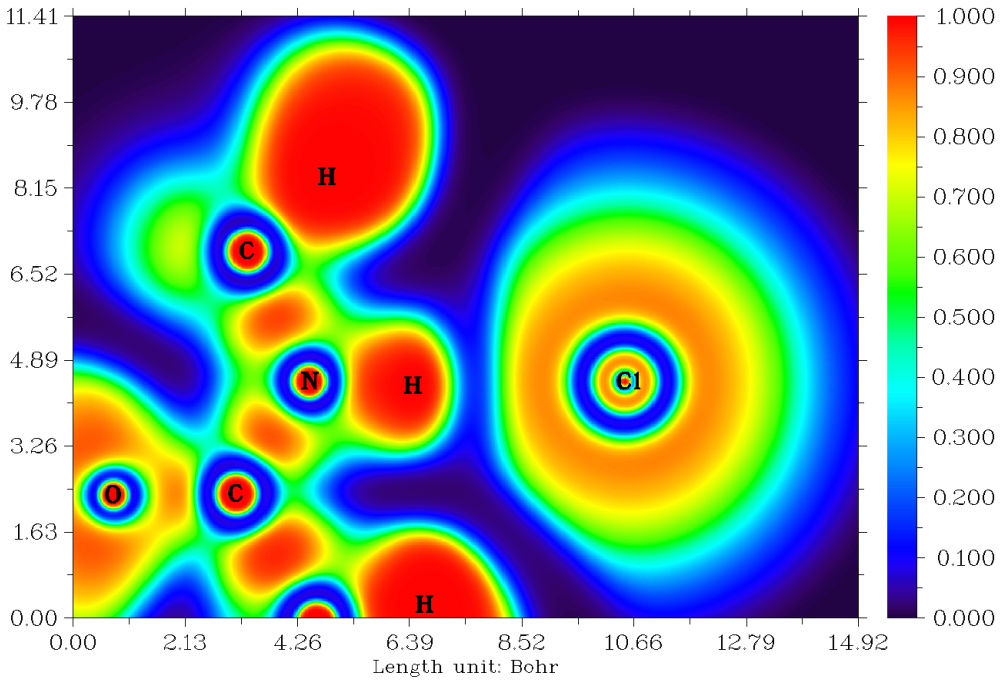

Figure S17: ELF of $Cl(NMA)^-$ in B3LYP/6-311+G** level of theory.

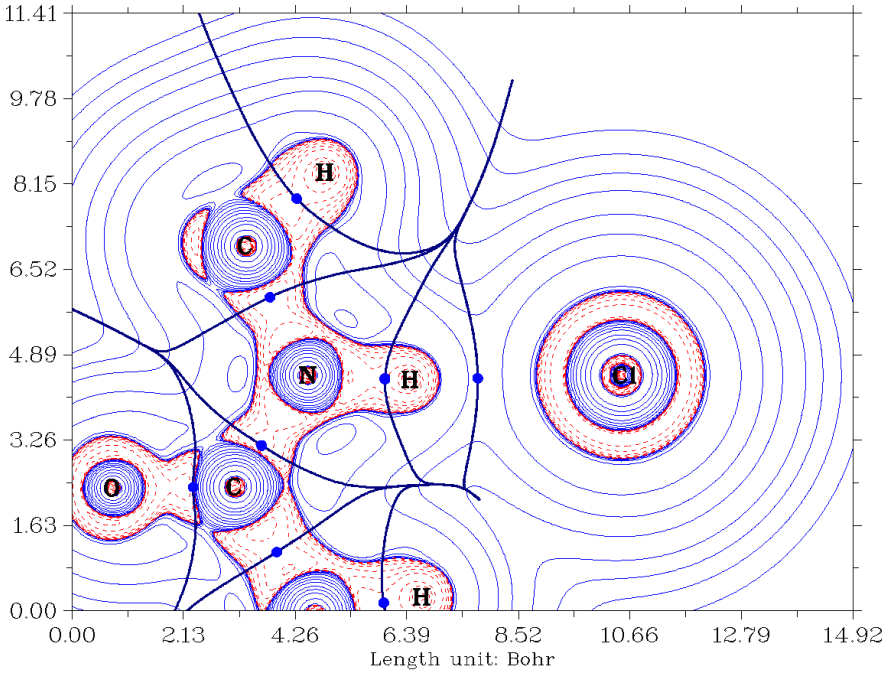

Figure S18: Laplacian of the electronic density of $Cl(NMA)_2^-$ in B3LYP/6-311+G** level of theory; Blue lines laplacian value is positive, red line laplacian

value is negative, blue dots are critical point (3,-1) and black line are QTAIM basin area.

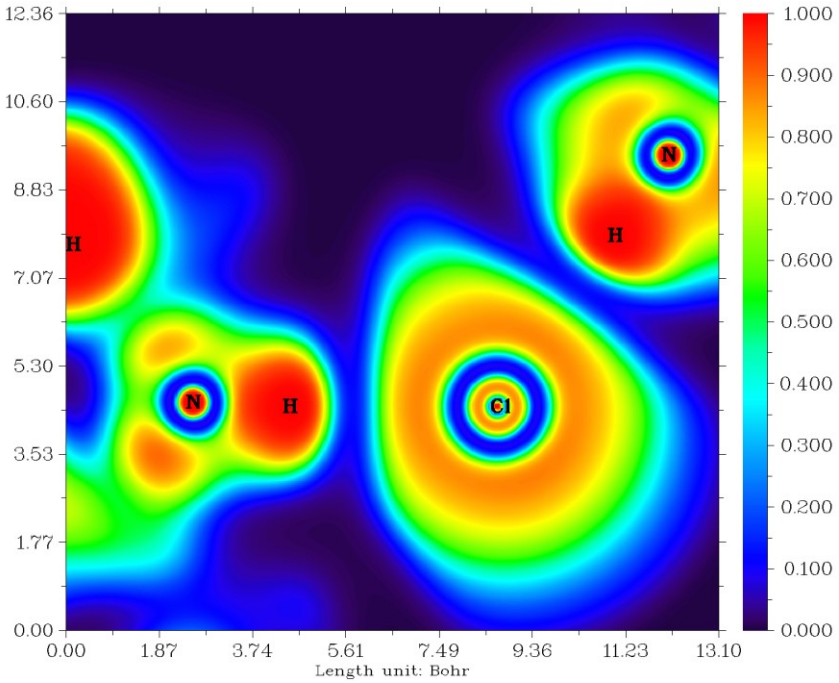

Figure S19: ELF of $Cl(NMA)_2^-$ in B3LYP/6-311+G** level of theory.

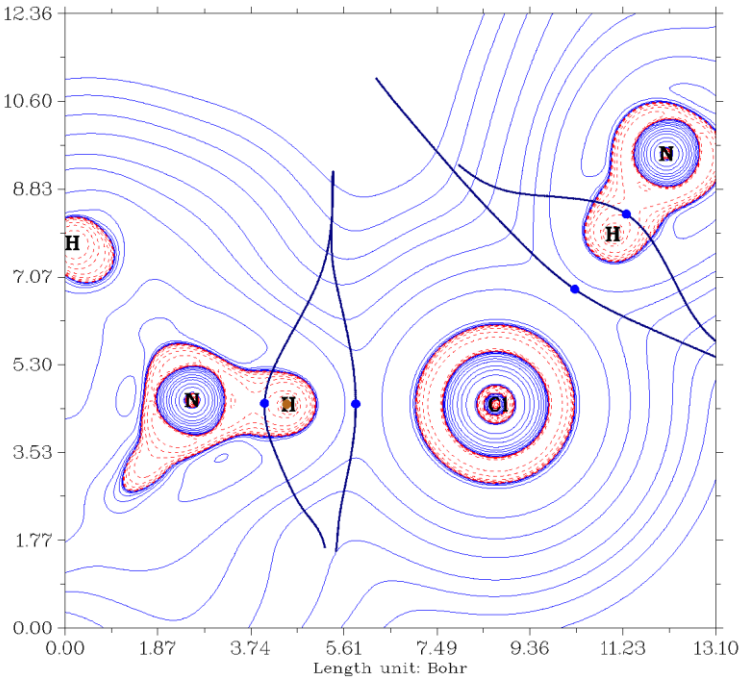

Figure S20: Laplacian of the electronic density of $Cl(NMA)_2^-$ in B3LYP/6-311+G** level of theory; Blue lines laplacian value is positive, red line laplacian value is negative, blue dots are critical point (3,-1) and black line are QTAIM basin area.

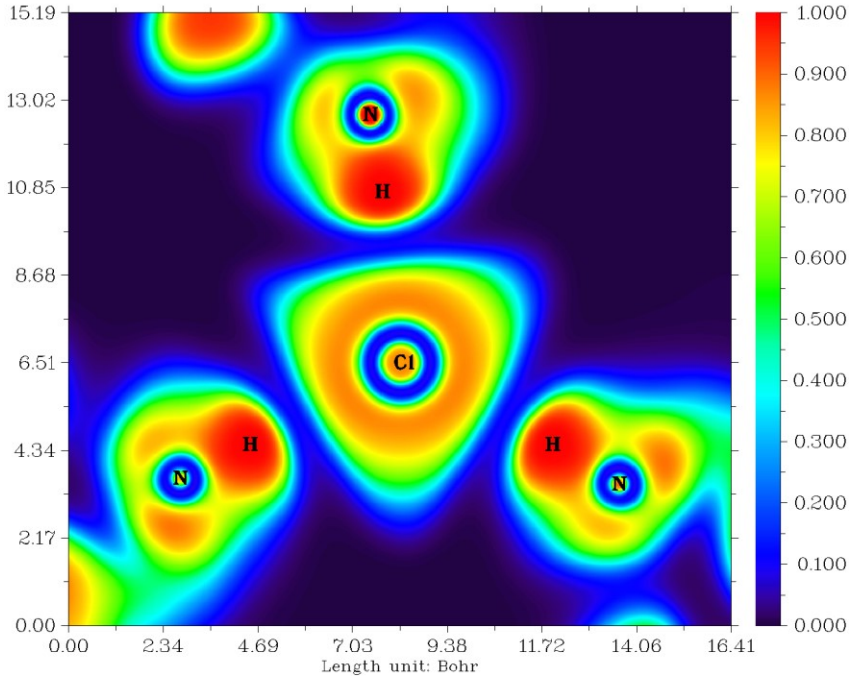

Figure S21: ELF of $Cl(NMA)_3^-$ in B3LYP/6-311+G** level of theory.

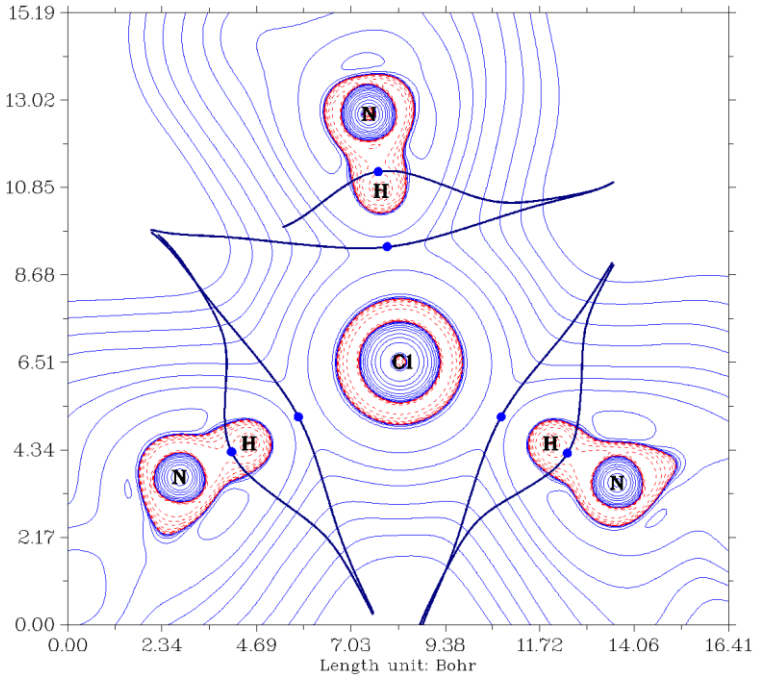

Figure S22: Laplacian of the electronic density of $Cl(NMA)_3^-$ in B3LYP/6-311+G** level of theory; Blue lines laplacian value is positive, red line laplacian value is negative, blue dots are critical point (3,-1) and black line are QTAIM basin area.

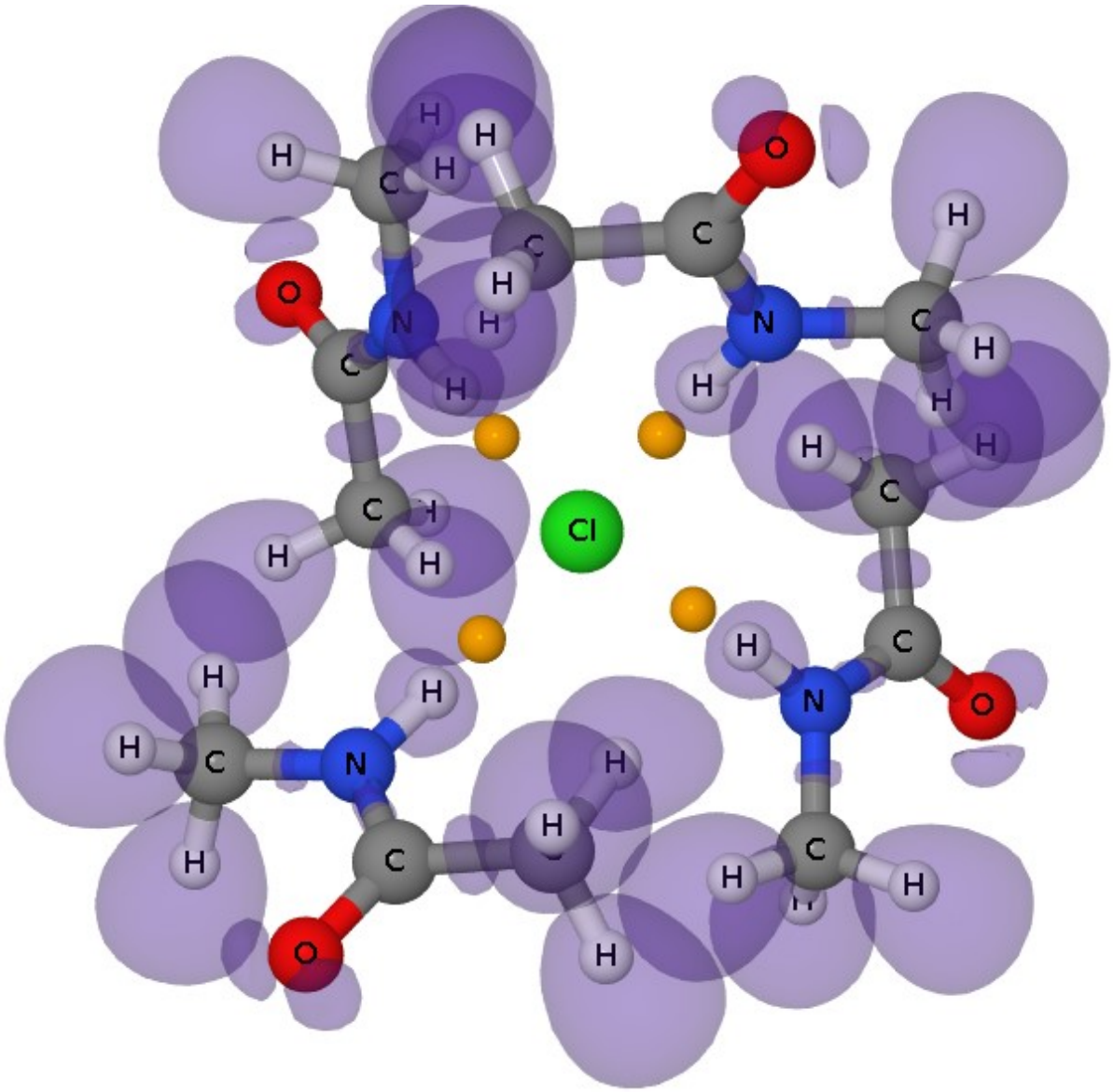

Figure S23: isosurface of 0.85 of the ELF of $Cl(NMA)_4^-$ in B3LYP/6-311+G** level of theory and critical point (3,-1) in orange.

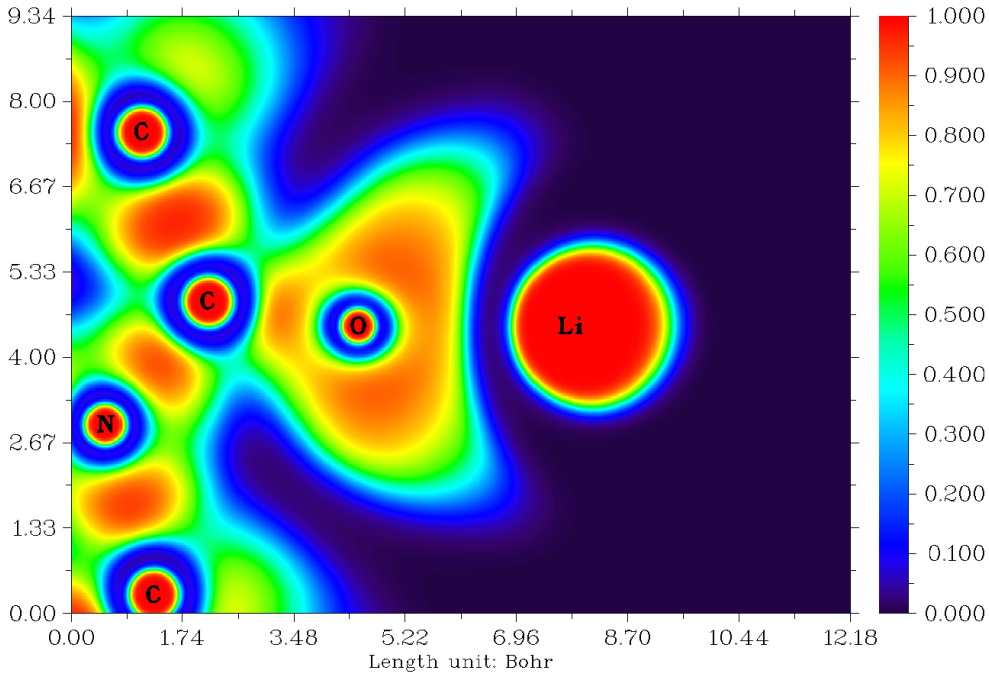

Figure S24: ELF of $Li(NMA)^+$ in B3LYP/6-311+G** level of theory.

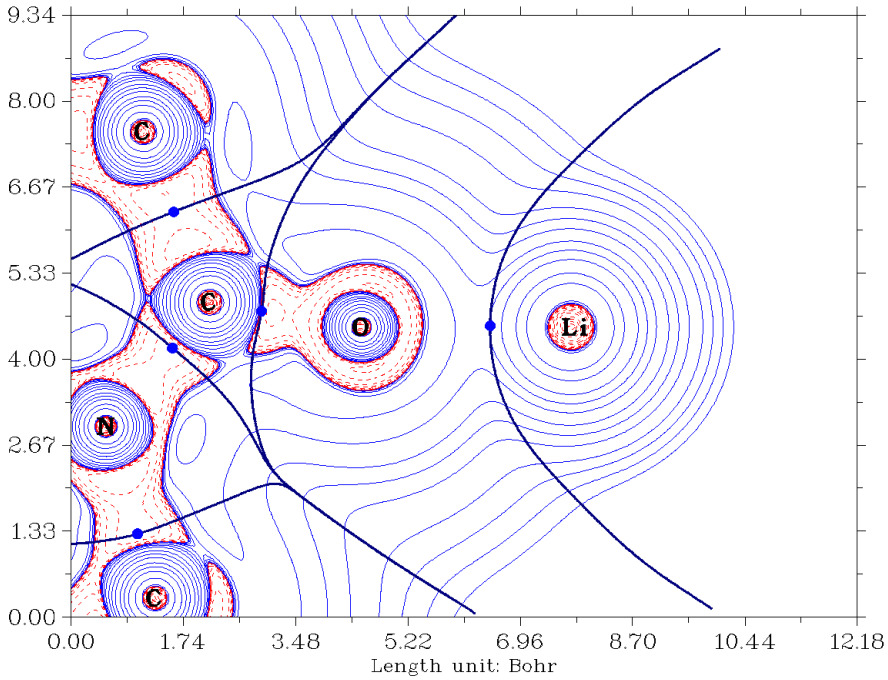

Figure S25: Laplacian of the electronic density of $Li(NMA)^+$ in B3LYP/6-311+G** level of theory; Blue lines laplacian value is positive, red line laplacian value is negative, blue dots are critical point (3,-1) and black line are QTAIM basin area.

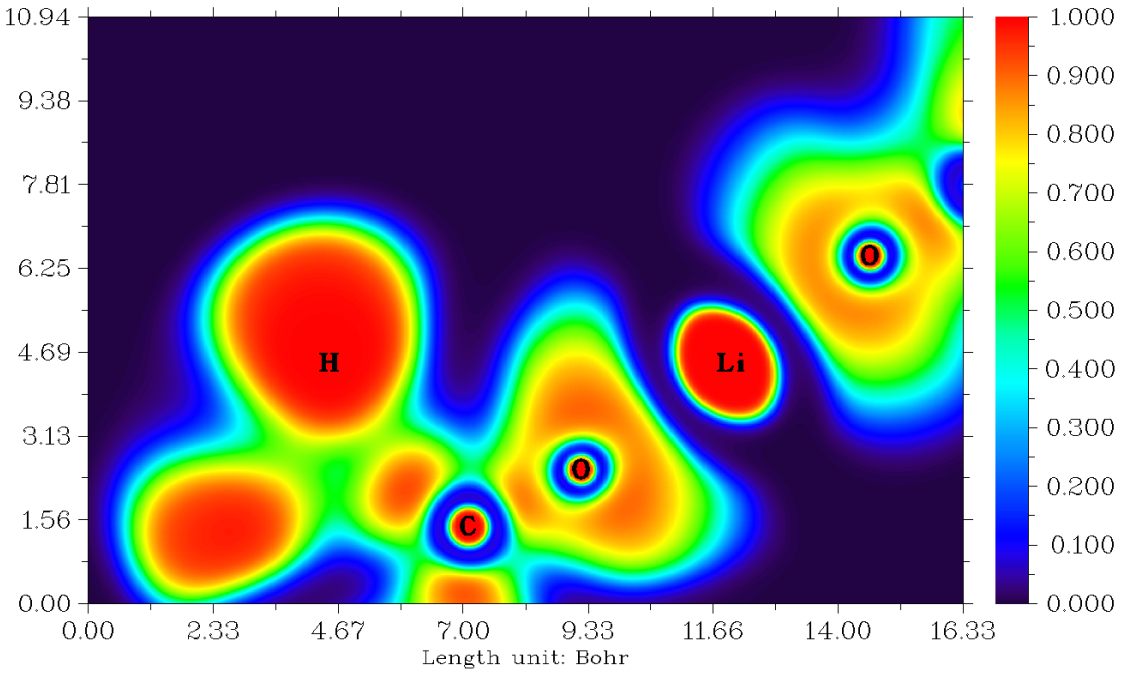

Figure S26: ELF of $Li(NMA)_2^+$ in B3LYP/6-311+G** level of theory.

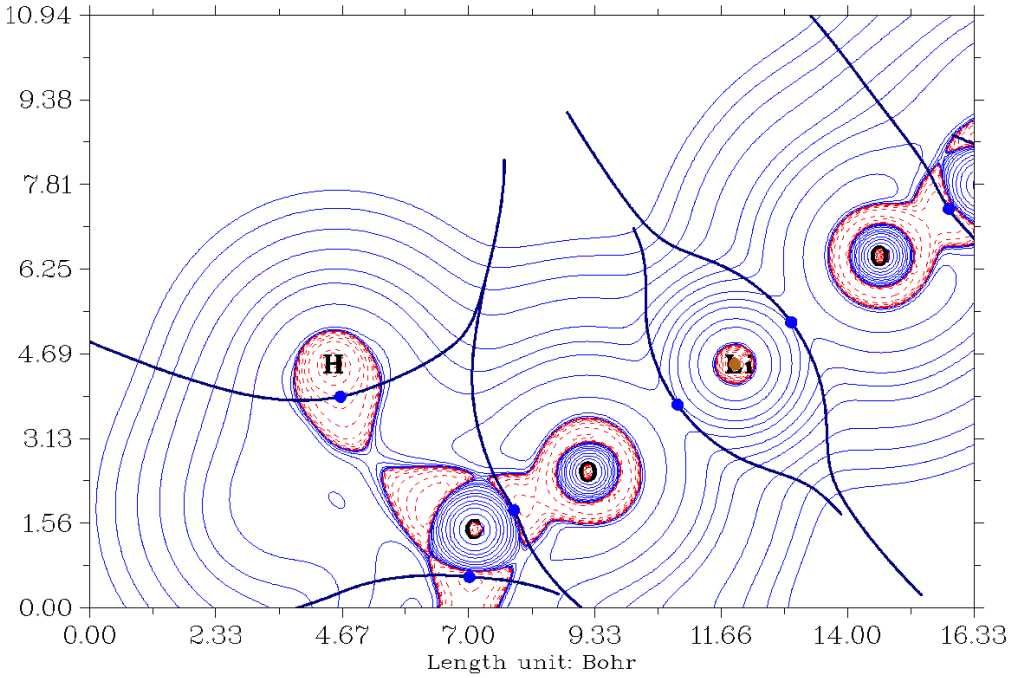

Figure S27: Laplacian of the electronic density of $Li(NMA)_2^+$ in B3LYP/6-311+G** level of theory; Blue lines laplacian value is positive, red line laplacian value is negative, blue dots are critical point (3,-1) and black line are QTAIM basin area.

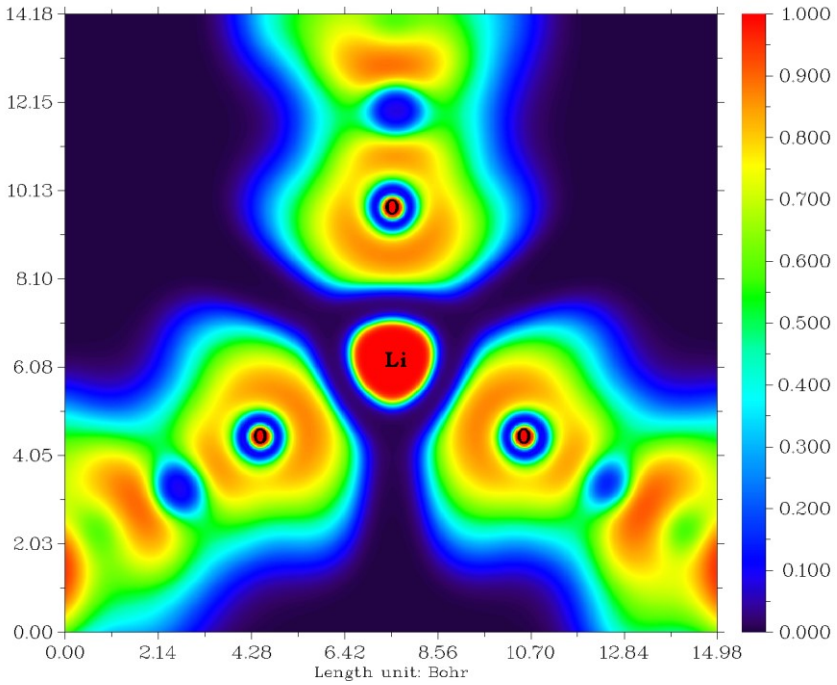

Figure S28: ELF of $Li(NMA)_3^+$ in B3LYP/6-311+G** level of theory.

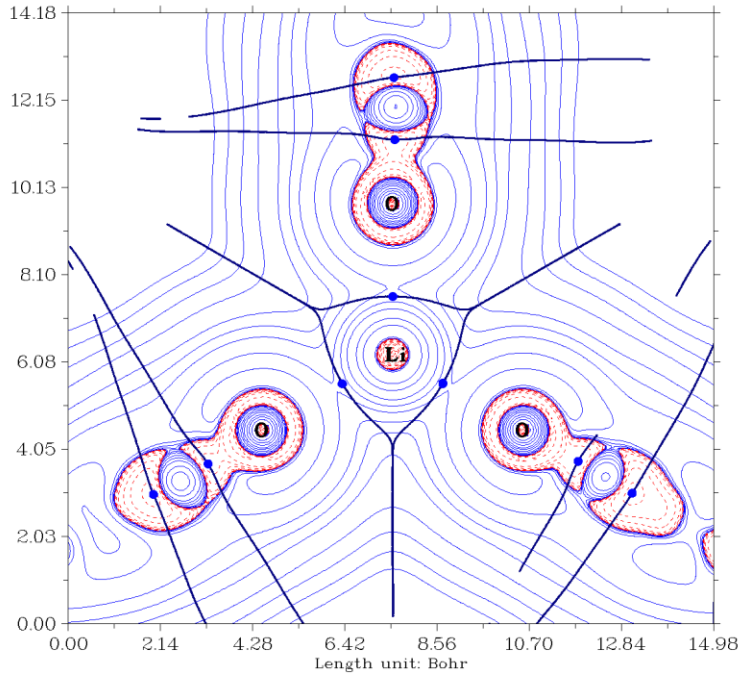

Figure S29: Laplacian of the electronic density of $Li(NMA)_3^+$ in B3LYP/6-311+G** level of theory; Blue lines laplacian value is positive, red line laplacian value is negative, blue dots are critical point (3,-1) and black line are QTAIM basin area.

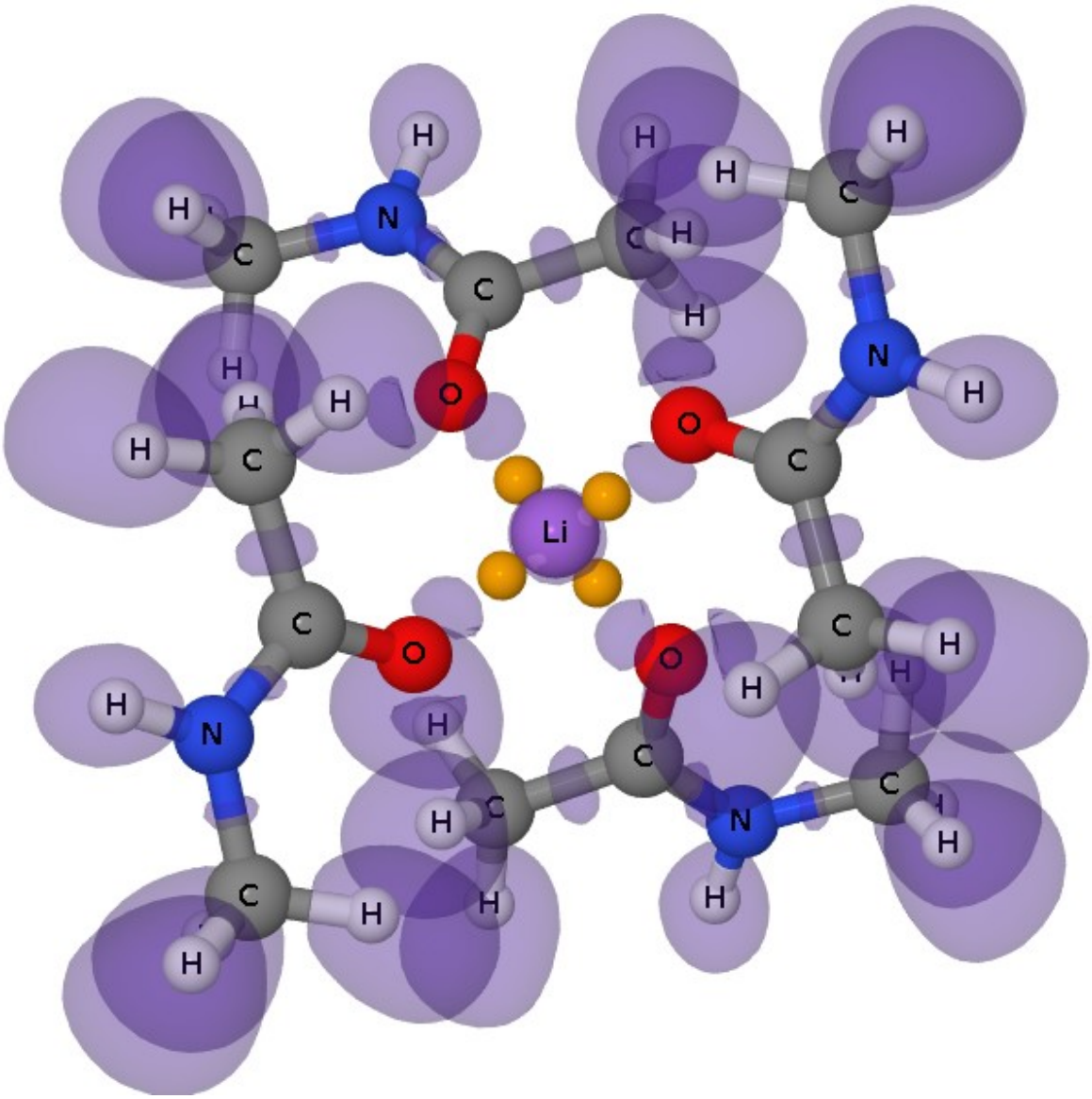

Figure S23: isosurface of 0.85 of the ELF of $Li(NMA)_4^+$ in B3LYP/6-311+G** level of theory and critical point (3,-1) in orange.