

Cold-Spray Ionization Mass Spectrometry of the Choline Chloride-Urea Deep Eutectic Solvent (Reline)

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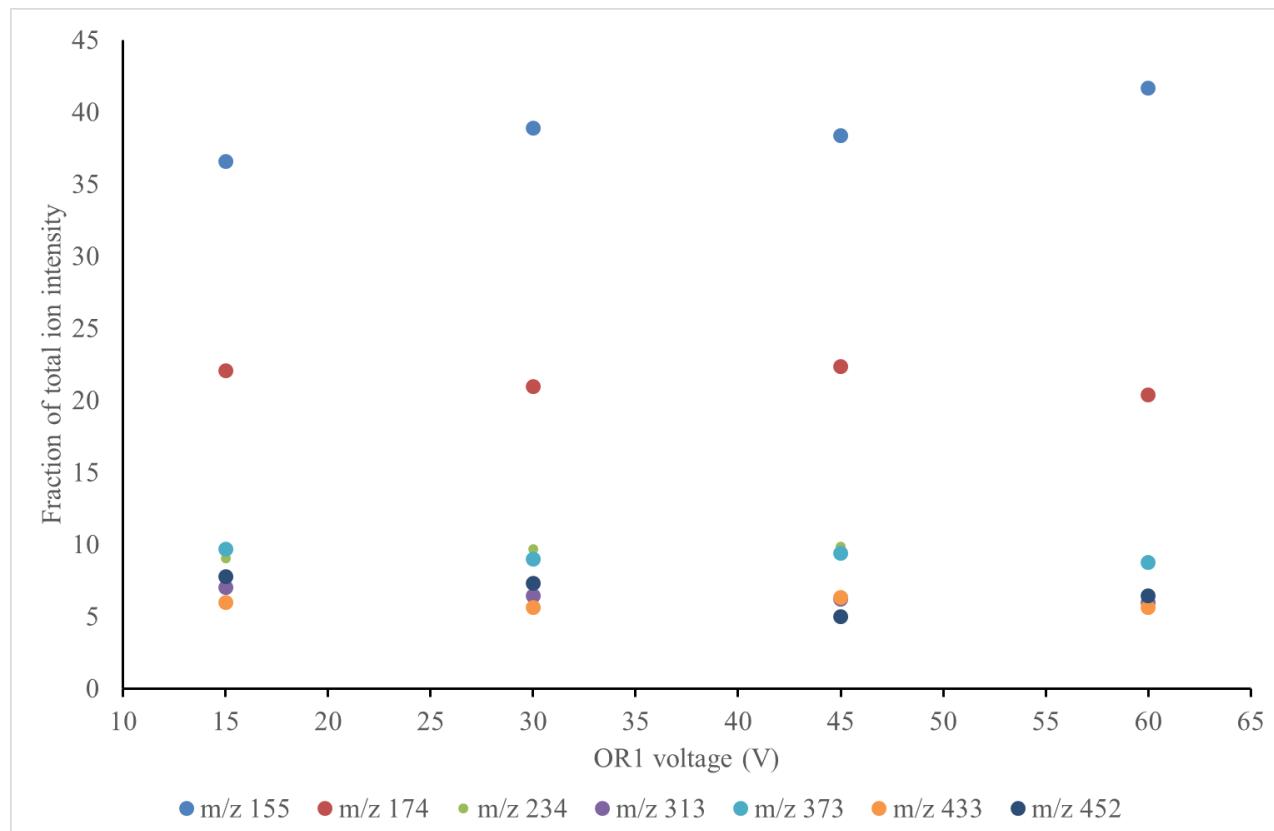


Figure S1 : Fractions of intensities of the ions $[(U)_2+Cl]^-$, $[(ChCl)_n+(U)_2+Cl]^-$, $[(ChCl)_n+U+Cl]^-$ and $[(ChCl)_n+Cl]^-$, and where $n = 1$ to 3 reported as a function of the orifice 1 voltage values, the OR2 voltage value being kept at 5V.

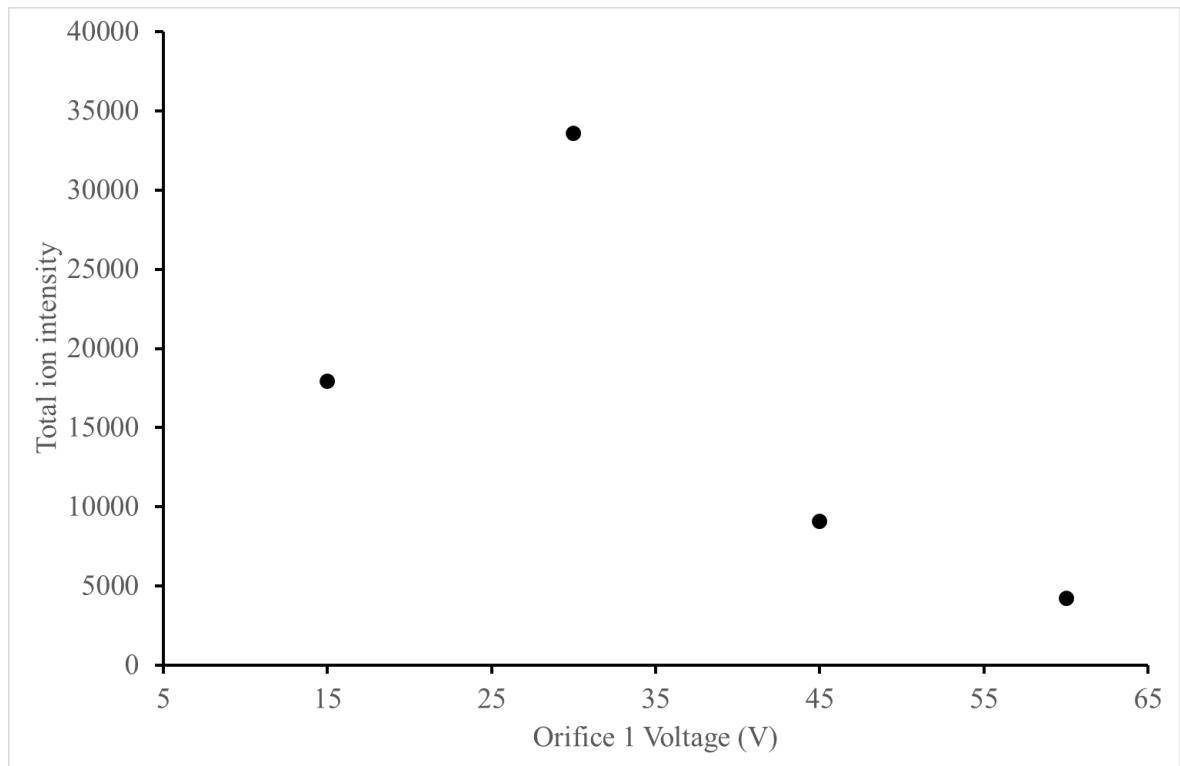


Figure S2 : Sum of the intensities of the ions $[(U)_2+Cl]^-$, $[(ChCl)_n+(U)_2+Cl]^-$, $[(ChCl)_n+U+Cl]^-$ and $[(ChCl)_n+Cl]^-$, and where $n = 1$ to 3 reported as a function of the orifice 1 voltage values, the OR2 voltage value being kept at 5V.

Table S1 : B3LYP/6-311++G(d,p) energies (in hartrees) of the isolated species

Cl ⁻	-460.3037
Urea	-225.3560
Choline	-328.8206
Ch:Cl	-789.2825 (with OH ⁻ ...Cl interaction) -789.2704 (with Methyl ⁻ ...Cl interaction)
U:Cl	-685.7040

Table S2: Total energy E_{total} (in hartrees), interaction energies (ΔE , in $\text{kJ}.\text{mol}^{-1}$), relative interaction energies (ΔE_{rel} , in $\text{kJ}.\text{mol}^{-1}$) and structures after QM E(B3LYP/6-311++G(d,p) geometry optimization for different minima of the $m/z = 155$ anion.

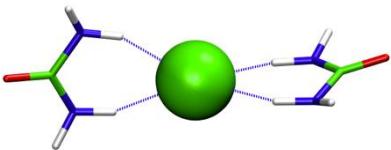
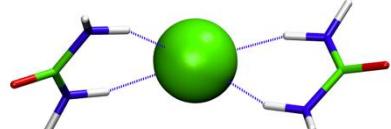
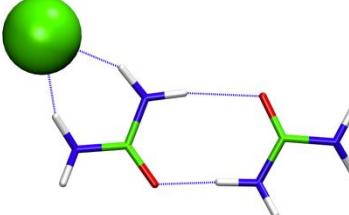
<i>m/z 155</i>	E_{total} (hartree)	ΔE ($\text{kJ}.\text{mol}^{-1}$)	ΔE_{rel} ($\text{kJ}.\text{mol}^{-1}$)	Optimized structures
A	-911.0962	-210.7	0.0	
B	-911.0961	-210.7	0.1	
C	-911.0822	-174.3	36.6	

Table S3 : Total energy E_{total} (in hartrees), interaction energies (ΔE , in $\text{kJ}.\text{mol}^{-1}$), relative interaction energies (ΔE_{rel} , in $\text{kJ}.\text{mol}^{-1}$) and structures after QM E(B3LYP/6-311++G(d,p) geometry optimization for different minima of the $m/z = 234$ anion.

m/z 234	E_{total} (hartree)	ΔE ($\text{kJ}.\text{mol}^{-1}$)	ΔE_{rel} ($\text{kJ}.\text{mol}^{-1}$)	Optimized structures
A	-1475.0335	-654.2	6.1	
B	-1475.0345	-656.9	3.3	
C	-1475.0353	-658.9	1.3	
D	-1475.0358	-660.3	0.0	
E	-1475.0348	-657.5	2.8	
F	-1475.0325	-651.7	8.6	

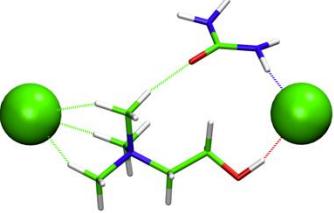
G	-1475.0132	-600.9	59.3	
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Table S3: Total energy E_{total} (in hartrees), interaction energies (ΔE , in $\text{kJ}\cdot\text{mol}^{-1}$), relative interaction energies (ΔE_{rel} , in $\text{kJ}\cdot\text{mol}^{-1}$) and structures after QM E(B3LYP/6-311++G(d,p) geometry optimization for different minima of the $m/z = 294$ anion.

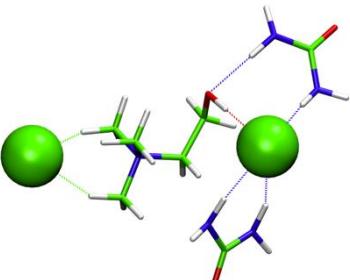
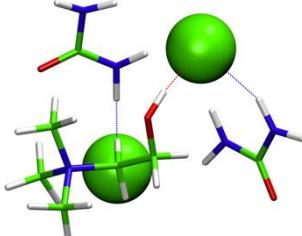
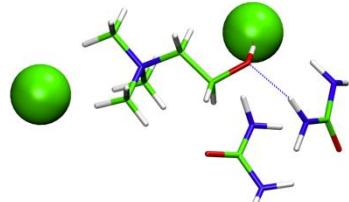
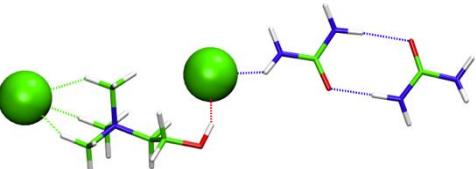
m/z 294	E_{total} (hartree)	ΔE ($\text{kJ}\cdot\text{mol}^{-1}$)	ΔE_{rel} ($\text{kJ}\cdot\text{mol}^{-1}$)	Optimized structures
A	-1700.4180	-728.8	0.0	
B	-1700.4009	-684.0	44.9	
C	-1700.4159	-723.3	5.5	
D	-1700.3936	-664.8	64.0	

Table S4 : Total energy E_{total} (in hartrees), interaction energies (ΔE , in $\text{kJ}.\text{mol}^{-1}$), relative interaction energies (ΔE_{rel} , in $\text{kJ}.\text{mol}^{-1}$) and structures after QM E(B3LYP/6-311++G(d,p) geometry optimization for different minima of the $m/z = 373$ anion.

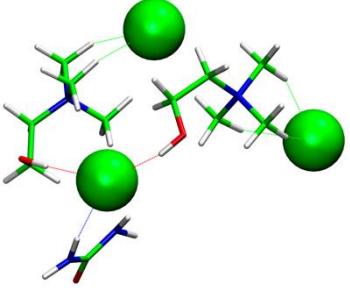
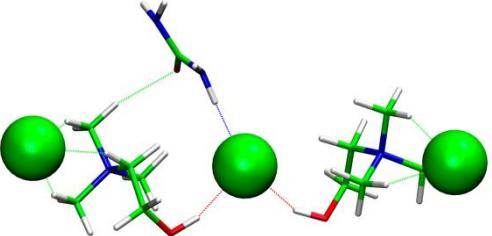
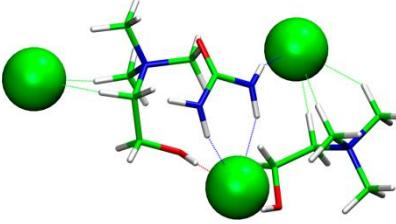
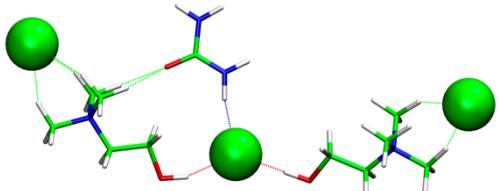
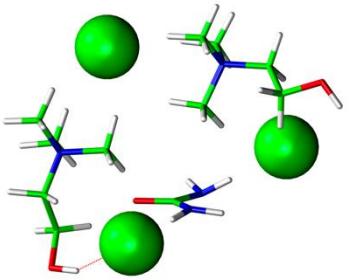
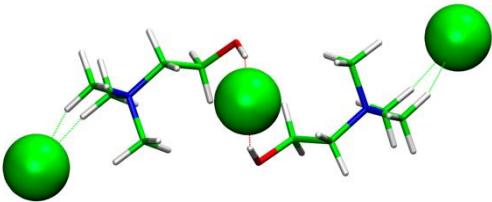
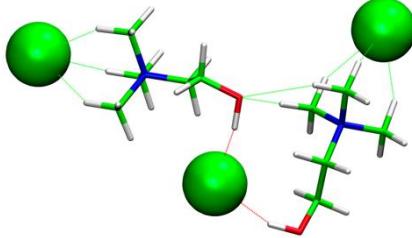
m/z 373	E_{total}	ΔE	ΔE_{rel}	Optimized structures
ChCl:U 1:2	(hartree)	($\text{kJ}.\text{mol}^{-1}$)	($\text{kJ}.\text{mol}^{-1}$)	
A	-2264.3547	-1170.6	0.0	
B	-2264.3344	-1117.3	53.2	
C	-2264.3539	-1168.5	2.1	
D	-2264.3341	-1116.6	54.0	
E	-2264.3390	-1129.4	41.2	

Table S5: Total energy E_{total} (in hartrees), interaction energies (ΔE , in $\text{kJ}\cdot\text{mol}^{-1}$), relative interaction energies (ΔE_{rel} , in $\text{kJ}\cdot\text{mol}^{-1}$) and structures after QM E(B3LYP/6-311++G(d,p) geometry optimization for different minima of the $m/z = 373$ anion.

m/z 373	E_{total}	ΔE	ΔE_{rel}	Optimized structures
ChCl 2 :0	(hartree)	($\text{kJ}\cdot\text{mol}^{-1}$)	($\text{kJ}\cdot\text{mol}^{-1}$)	
A	-2038.9596	-1068.1	0.0	
B	-2038.9585	-1065.2	2.9	
C	-2038.9582	-1064.5	3.7	