Speciation of La(III) chloride complexes in water and acetonitrile. A density functional study.

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Table S1: Computed BSSE corrections (kcal/mol). *(a)* nature of the small fragment considered in the counterpoise correction procedure. Two fragments were used, the other fragment is the rest of the complex. The global complex considered for the BSSE correction is specified in the "In complex" column.[a]

Fragment[b]	In complex	BSSE correction (kcal/mol)
	Ninefold coordinated complexes [c]	
H_2O	**0.9.0**	1.9
MeCN	**0.0.9**	0.8
Cl^-	**1.8.0**	1.0
	Eightfold coordinated complexes [c]	
H_2O	**0.8.0**	1.9
MeCN	**0.0.8**	0.6
Cl^-	**1.7.0**	1.0
	Sevenfold coordinated complexes [c]	
H_2O	**0.7.0**	1.8
MeCN	**0.0.7**	0.7
Cl^-	**1.6.0**	0.9

a. BLYP/SDD/6-311+G** single point energies on BLYP/SDD/6-31G** gas phase optimized structures.
b. Counterpoise corrections considering two fragments. The first fragment is either H_2O, MeCN or Cl^-, the second fragment is the rest of the complex
c. Slightly different BSSE corrections have been computed for nine-, eight- and seven-fold coordinated complexes.

Table S2: Energies (kcal/mol) for $LaCl_4^- \rightarrow LaCl_3 + Cl^-$

	ΔE	**ΔH**
Exp [a]		79.3 ± 2
Gaussian (SDD/6-311+G//SDD-6-31G*)**	75.0	
CP-opt (80 Ry)	74.2	
CP-opt (100 Ry)	73.3	

[a] Derived from $\Delta_r H^o(218.15K)$ for the gas-phase reactions $LuCl_4^-(g) \rightarrow LuCl_3(g) + Cl^-(g)$ and $LaCl_4^- + LuCl_3 \rightarrow LaCl_3 + LuCl_4^-$ (cf. L. S. Kudin, D. E. Vorob'ev, A. E. Grishin, *Russ. J. Phys. Chem. A* **2007**, *81*, 147-158).

Table S3a: Atomic charges (in *e*) from Natural Population Analysis [(a)]

Sevenfold coordinated complexes

	0.7.0	**1.6.0**	**2.5.0**	**3.4.0**
La^{3+}	+2.01	+1.63	+1.33	+1.14
O_{H2O}	-0.94	-0.92	-0.91	-0.89
H_{H2O}	+0.54	+0.53	+0.52	+0.51
H_2O	+0.14	+0.13	+0.13	+0.12
Cl^-	-	-0.42	-0.49	-0.54

Table S3b: Mulliken Atomic charges (in *e*) [(a)]

Ninefold coordinated complexes

	0.9.0	**1.8.0**	**2.7.0**	**3.6.0**
La^{3+}	+2.45	+1.76	+1.28	+0.94
O_{H2O}	-0.63	-0.59	-0.50	-0.43
H_{H2O}	+0.34	+0.33	+0.30	+0.28
H_2O	+0.06	+0.08	+0.09	+0.13
Cl^-	-	-0.36	-0.45	-0.57

Eightfold coordinated complexes

	0.8.0	**1.7.0**	**2.6.0**	**3.5.0**
La^{3+}	+2.22	+1.62	+1.14	+0.69
O_{H2O}	-0.61	-0.58	-0.51	-0.39
H_{H2O}	+0.35	+0.33	+0.30	+0.27
H_2O	+0.10	+0.09	+0.10	+0.14
Cl^-	-	-0.26	-0.37	-0.46

Sevenfold coordinated complexes

	0.7.0	**1.6.0**	**2.5.0**	**3.4.0**
La^{3+}	+2.04	+1.52	+1.15	+0.77
O_{H2O}	-0.59	-0.57	-0.53	-0.43
H_{H2O}	+0.36	+0.34	+0.31	+0.28
H_2O	+0.14	+0.11	+0.10	+0.13
Cl^-	-	-0.20	-0.34	-0.42

(a) BLYP/gas level (6-311+G** basis).

Table S4: Geometrical and electronic parameters describing the orientation of H_2O ligands in La^{3+} hydrates in the gas phase, in the three studied solvents (acetonitrile, water and [dmim][Cl])

	Gas phase (CP-Opt)		
	La-O (Å)	**μ (D)**	**θ_{tilt} (deg)**
0.9.0	2.65(1)	3.31(3)	177.4(12)
1.8.0	2.67(1)	3.07(6)	156.3(83)
0.8.0	2.61(0)	3.48(2)	178.0(7)
1.7.0	2.65(2)	3.17(5)	162.3(86)
2.6.0	2.67(3)	2.89(3)	138.6(80)
3.5.0	2.68(2)	2.67(3)	115.7(11)

	In acetonitrile [(a)]		
	La-O (Å)	**μ (D)**	**θ_{tilt} (deg)**
0.9.0, 3 Cl^-	2.65(13)	3.32(34)	150.4(152)
0.8.0, 0 Cl^-	2.60(11)	3.41(27)	154.8(140)
0.8.0, 3 Cl^-	2.65(14)	3.24(32)	146.9(182)
2.6.0, 1 Cl^-	2.68(16)	3.23(31)	149.9(184)
3.5.0, 0 Cl^-	2.68(15)	3.05(36)	138.1(232)

	In water [(a)]		
	La-O (Å)	**μ (D)**	**θ_{tilt} (deg)**
0.9.0, 3 Cl^-	2.65(15)	3.44(32)	151.4(166)
0.8.0, 0 Cl^-	2.60(13)	3.53(35)	150.2(152)
0.8.0, 3 Cl^-	2.58(12)	3.59(34)	159.7(117)
1.7.0, 2 Cl^-	2.60(12)	3.56(29)	153.4(142)
2.6.0, 1 Cl^-	2.62(14)	3.52(35)	147.7(154)
3.5.0, 0 Cl^-	2.61(10)	3.49(28)	151.0(147)

	In [dmim][Cl] [(b)]		
	La-O (Å)	**μ (D)**	**θ_{tilt} (deg)**
3.5.0	2.67(19)	3.30(42)	139.0(18)

(a) Averages over 1 ps of MD. (b) Averages over 13 snapshots.

Table S5: Energy components corresponding to Table 4.

	Gas			Acetonitrile		Water		Gas	Acet.	Water
	ΔE_{gas}	δE_G	δE_{BSSE}	ΔE_{soln}	δG_{nes}	ΔE_{soln}	δG_{nes}	ΔG_{gas}	ΔG_{PCM}	ΔG_{PCM}
0.9.0 + 1 Cl^- → **1.8.0** + 1 H_2O	-251.5	-2.3	-0.9	3.7	0.9	7.4	1.2	-254.7	1.4	5.4
0.9.0 + 2 Cl^- → **2.7.0** + 2 H_2O	-432.4	-4.2	-1.7	0.1	1.9	7.8	2.5	-438.3	-3.9	4.4
0.9.0 + 3 Cl^- → **3.6.0** + 3 H_2O	-539.6	-6.5	-2.6	3.2	2.9	7.7	3.8	-548.6	-2.9	2.5
0.8.0 + 1 Cl^- → **1.7.0** + 1 H_2O	-258.1	-4.6	-0.9	-1.2	1.0	3.4	1.3	-263.6	-5.7	-0.8
0.8.0 + 2 Cl^- → **2.6.0** + 2 H_2O	-440.7	-6.0	-1.8	-1.3	2.4	5.0	3.0	-448.6	-6.8	0.1
0.8.0 + 3 Cl^- → **3.5.0** + 3 H_2O	-550.2	-8.0	-2.7	1.1	2.7	8.8	3.5	-561.0	-6.9	1.6
0.7.0 + 1 Cl^- → **1.6.0** + 1 H_2O	-268.9	-4.5	-0.9	-5.5	0.7	-2.7	0.9	-274.3	-10.2	-7.3
0.7.0 + 2 Cl^- → **2.5.0** + 2 H_2O	-457.6	-7.5	-1.8	-11.3	1.8	-4.6	2.3	-466.9	-18.8	-11.6
0.7.0 + 3 Cl^- → **3.4.0** + 3 H_2O	-568.8	-8.4	-2.7	-8.0	2.1	-1.2	2.7	-579.9	-17.0	-9.6

a $\Delta G_{gas} = \Delta E_{gas} + \delta E_G + \delta E_{BSSE}$ and $\Delta G_{PCM} = \Delta E_{soln} + \delta G_{nes} + \delta E_G + \delta E_{BSSE}$; see Computational Details for definitions of these terms.

Table S6: Energy components corresponding to Table 5.

	Gas			Acetonitrile		Water		Gas	Acet.	Water
	ΔE_{gas}	δE_G	δE_{BSSE}	ΔE_{soln}	δG_{nes}	ΔE_{soln}	δG_{nes}	ΔG_{gas}	ΔG_{PCM}	ΔG_{PCM}
0.9.0 + 9 MeCN → **0.0.9** + 9 H_2O	-94.8	-9.2	-9.8	37.8	14.6	38.2	18.5	-113.8	33.4	37.7
1.8.0 + 8 MeCN → **1.0.8** + 8 H_2O	-34.7	-8.0	-8.7	26.0	13.0	25.9	16.5	-51.4	22.4	25.7
2.7.0 + 7 MeCN → **2.0.7** + 7 H_2O	13.5	-7.4	-7.6	29.3	10.7	26.5	13.4	-1.6	24.9	24.9
3.6.0 + 6 MeCN → **3.0.6** + 6 H_2O	47.3	-8.9	-6.5	25.6	9.0	25.1	11.2	31.8	19.1	20.9
0.8.0 + 8 MeCN → **0.0.8** + 8 H_2O	-100.3	-6.3	-9.9	33.6	12.1	34.4	15.2	-116.5	29.5	33.4
1.7.0 + 7 MeCN → **1.0.7** + 7 H_2O	-41.8	-5.2	-8.7	22.7	10.7	22.5	13.4	-55.7	19.5	22.1
2.6.0 + 6 MeCN → **2.0.6** + 6 H_2O	0.3	-6.9	-7.4	15.3	8.6	15.4	10.8	-14.1	9.6	11.8
3.5.0 + 5 MeCN → **3.0.5** + 5 H_2O	*dissoc*	*dissoc*	*-6.2*	*dissoc*	*dissoc*	*dissoc*	*dissoc*	*dissoc*	*dissoc*	*dissoc*
0.7.0 + 7 MeCN → **0.0.7** + 7 H_2O	-105.6	-7.0	-7.7	30.3	9.3	29.0	11.5	-120.3	24.9	25.8
1.6.0 + 6 MeCN → **1.0.6** + 6 H_2O	-46.2	-6.7	-6.6	19.6	11.5	20.8	14.0	-59.5	17.8	21.6
2.5.0 + 5 MeCN → **2.0.5** + 5 H_2O	-5.7	-4.7	-5.5	14.2	6.6	13.4	8.0	-15.9	10.6	11.2
3.4.0 + 4 MeCN → **3.0.4** + 4 H_2O	18.8	-4.5	-4.4	7.3	4.6	8.3	5.7	9.9	3.0	5.0

a $\Delta G_{gas} = \Delta E_{gas} + \delta E_G + \delta E_{BSSE}$ and $\Delta G_{PCM} = \Delta E_{soln} + \delta G_{nes} + \delta E_G + \delta E_{BSSE}$; see Computational Details for definitions of these terms. *dissoc* indicates that one ligand dissociates from one of the reaction partner during gas-phase optimizations.

Table S7: Energy components corresponding to Table 6.

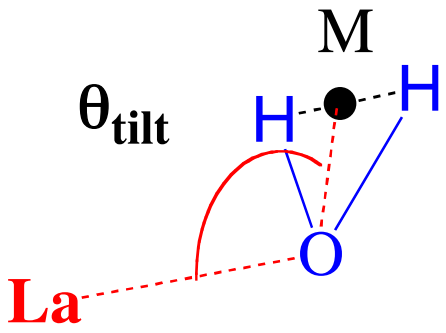
	Gas			Acetonitrile		Water	
	ΔE_{gas}	δE_G	δE_{BSSE}	ΔE_{soln}	δG_{nes}	ΔE_{soln}	δG_{nes}
0.9.0 → **0.8.0** + H_2O	21.9	-6.0	-1.9	8.8	2.6	7.7	2.7
0.8.0 → **0.7.0** + H_2O	29.8	-7.5	-1.9	13.1	2.5	13.6	2.6
3.6.0 → **3.5.0** + H_2O	11.2	-7.6	-1.9	6.6	2.4	8.7	2.4
3.5.0 → **3.4.0** + H_2O	11.3	-7.9	-1.9	4.1	1.9	3.5	1.9
3.6.0 + MeCN → **3.4.1** + 2 H_2O	20.4	-8.5	-3.0	16.7	3.8	18.1	4.2

a $\Delta G_{gas} = \Delta E_{gas} + \delta E_G + \delta E_{BSSE}$ and $\Delta G_{PCM} = \Delta E_{soln} + \delta G_{nes} + \delta E_G + \delta E_{BSSE}$; see Computational Details for definitions of these terms.

Table S8: Energies components and Free energies (kcal/mol) for reactions involved in the speciation histogram (see Figure S**).

	GAS			MeCN		H_2O		GAS	MeCN	H_2O
	ΔE Gas	**ΔE_G**	**ΔE_{bsse}**	**ΔE_{soln}**	**ΔG_{nes}**	**ΔEsoln**	**ΔG_{nes}**	**ΔG**	**ΔG**	**ΔG**
0.9.0 + 1 Cl^- → **1.8.0** + 1 H_2O	-251.5	-2.3	-0.9	3.7	0.9	7.4	1.2	-254.7	1.4	5.4
0.9.0 + 2 Cl^- → **2.7.0** + 2 H_2O	-432.4	-4.2	-1.7	0.1	1.9	7.8	2.5	-438.3	-3.9	4.4
0.9.0 + 3 Cl^- → **3.6.0** + 3 H_2O	-539.6	-6.5	-2.6	3.2	2.9	7.7	3.8	-548.6	-2.9	2.5
0.9.0 + 3 Cl^- → **0.8.0** + 1 H_2O + 3 Cl^-	21.9	-6.0	-1.9	8.8	2.6	7.7	2.7	14.0	3.4	2.4
0.9.0 + 3 Cl^- → **1.7.0** + 2 H_2O + 2 Cl^-	-236.2	-10.6	-2.8	7.6	3.6	11.1	3.9	-249.6	-2.3	1.6
0.9.0 + 3 Cl^- → **2.6.0** + 3 H_2O + 1 Cl^-	-418.8	-12.1	-3.7	7.5	4.9	12.7	5.7	-434.6	-3.4	2.6
0.9.0 + 3 Cl^- → **3.5.0** + 4 H_2O + 0 Cl^-	-528.3	-14.0	-4.6	9.9	5.3	16.5	6.2	-547.0	-3.5	4.0
0.9.0 + 3 Cl^- → **0.7.0** + 2 H_2O + 3 Cl^-	51.7	-13.6	-3.8	21.9	5.1	21.2	5.3	34.4	9.6	9.2
0.9.0 + 3 Cl^- → **1.6.0** + 3 H_2O + 2 Cl^-	-217.1	-18.1	-4.7	16.4	5.8	18.5	6.3	-239.9	-0.6	2.0
0.9.0 + 3 Cl^- → **2.5.0** + 4 H_2O + 1 Cl^-	-405.9	-21.1	-5.6	10.7	6.9	16.7	7.6	-432.5	-9.1	-2.4
0.9.0 + 3 Cl^- → **3.4.0** + 5 H_2O + 0 Cl^-	-517.0	-21.9	-6.5	13.9	7.2	20.0	8.1	-545.4	-7.3	-0.3

(a) BSSE corrections: -1.9 kcal/mol (H_2O) and +1.0 kcal/mol (Cl^-)



Scheme S1: Definition of tilt angle θ_{tilt} .

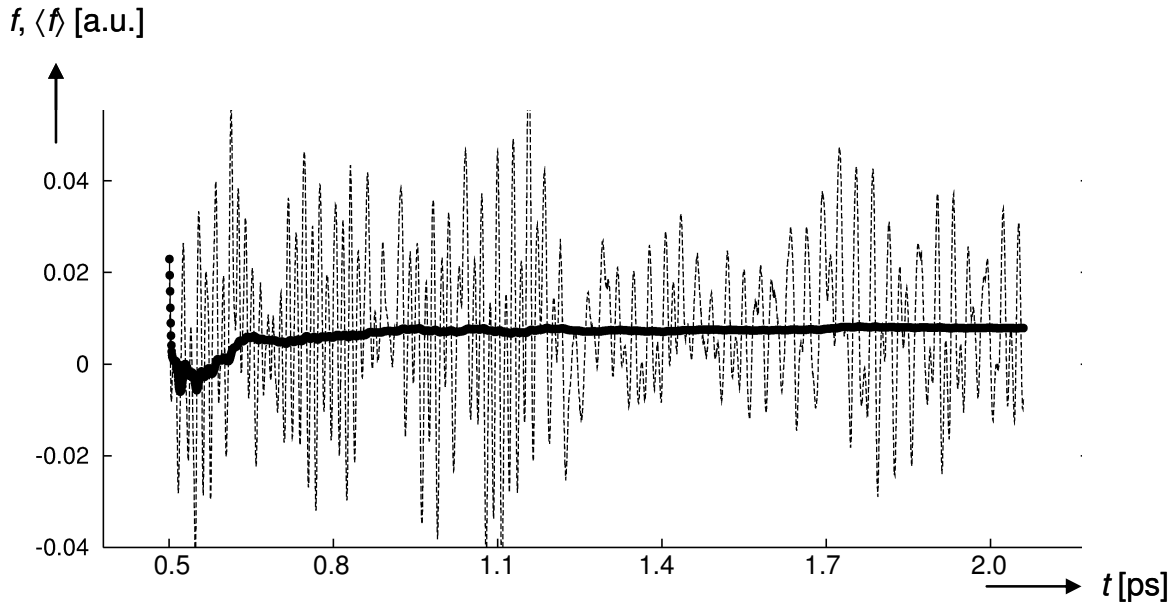


Figure S1: Convergence of the mean constraint force $\langle f \rangle$ (filled circles), obtained as the running (cumulative) average over the instantaneous forces f (dashed line) after 0.5 ps of equilibration; illustrative result from one CPMD run from the dissociation of one water ligand in **0.9.0** in aqueous solution (left in Figure 1 in the main paper) with fixed r = 3.75 Å. The converged value of $\langle f \rangle$ = 0.00784(27) a.u. (in parentheses: standard deviation during the last picosecond).

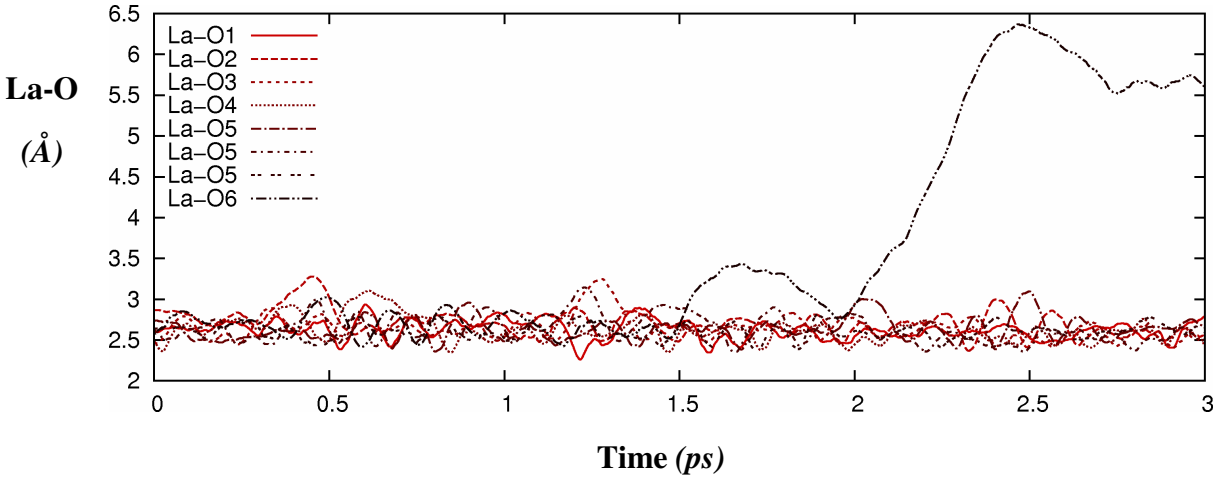
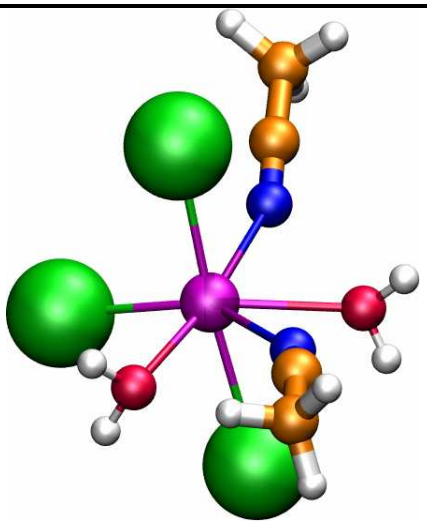
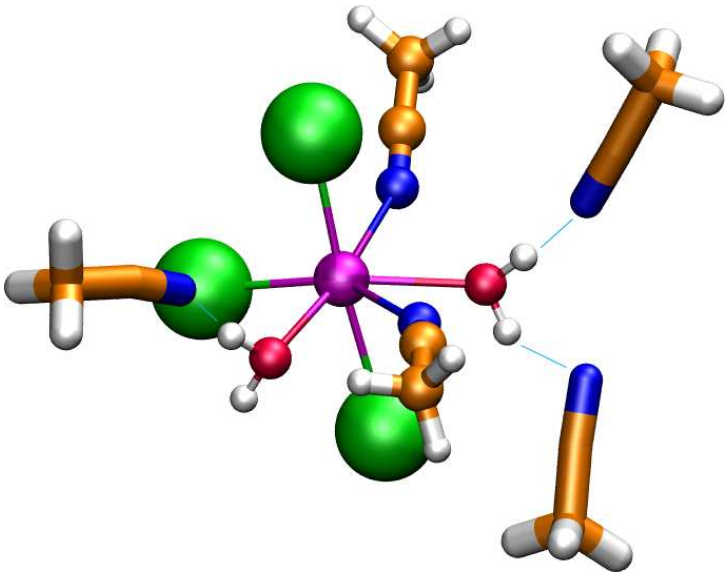


Figure S2: Time evolution of La-O distances (Å) in aqueous **1.8.0·(2Cl$^-$)** starting from the endpoint of the second PTI path.



3.2.2 in acetonitrile (complex only)



3.2.2 in acetonitrile (complex + second shell MeCN)

Figure S3: Snapshots of **3.2.2** in acetonitrile. Top: only the complex is shown. Bottom: view of the complex including interacting second shell acetonitrile molecules.

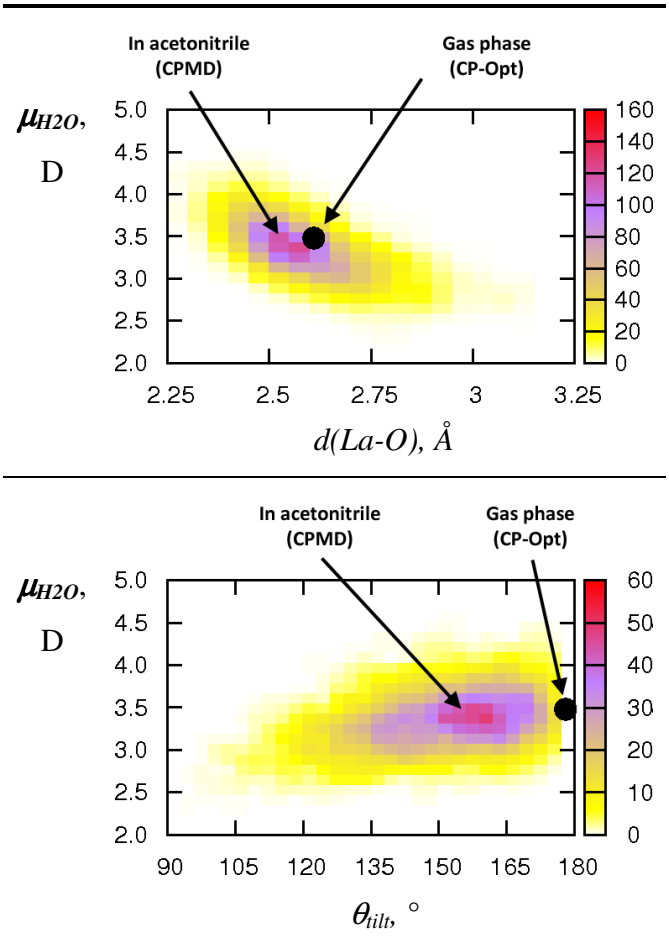


Figure S4: Scatter plots of the dipole moments of aquo ligands vs. selected geometrical parameters along CPMD trajectories in acetonitrile, considering **0.8.0** in absence of Cl^- counterions (see Scheme S1 for definition of θ_{tilt}): results are shown as density maps in rectangular bins, (color-coded according to occurrences over the last 7.6 ps of MD / 788 snapshots).

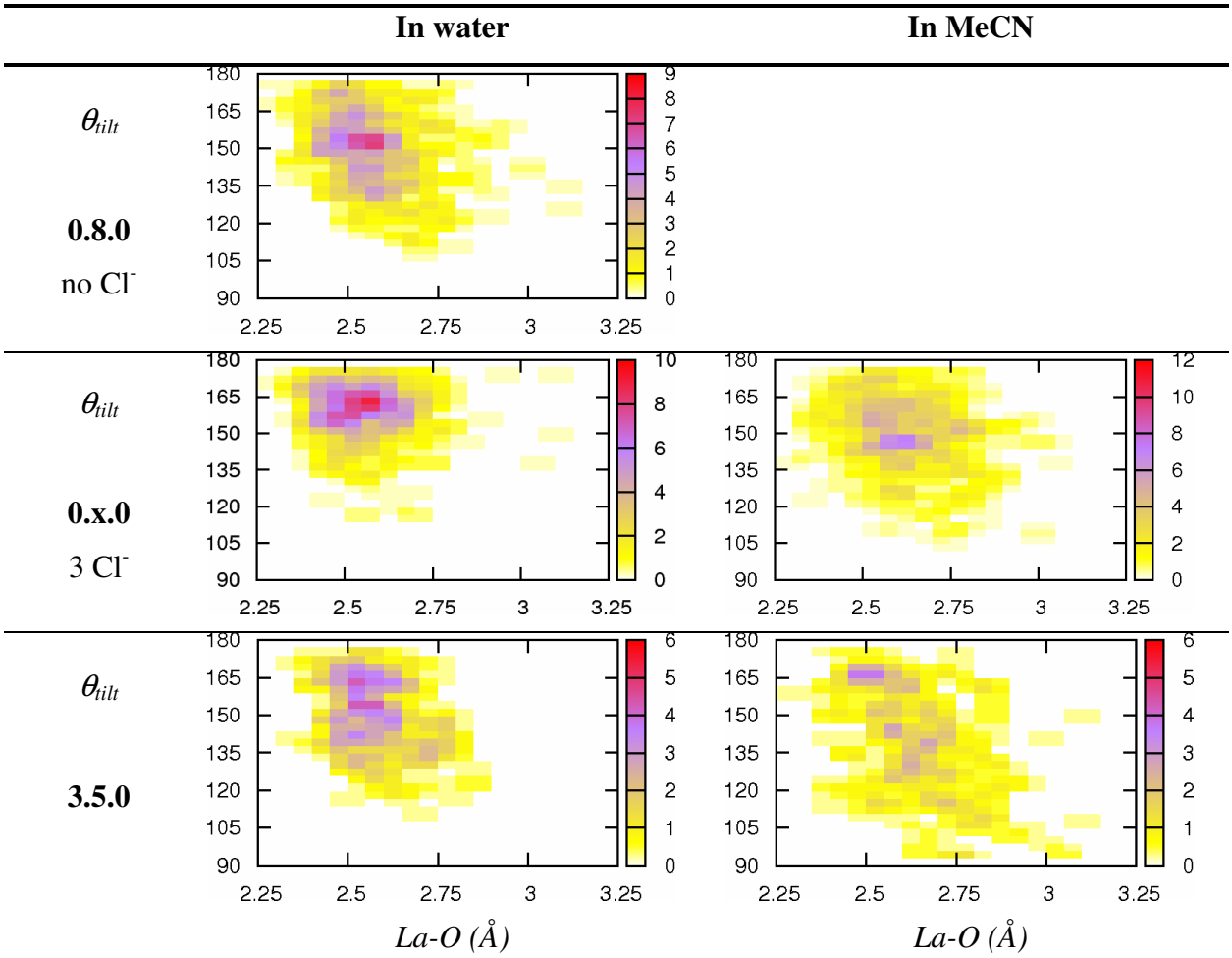


Figure S5: Correlation between La-O distances and θ_{tilt} angles (°) along CPMD trajectories (see Scheme S1 for definition of θ_{tilt}): results are shown as density maps in rectangular bins, (color-coded according to occurrences over 50 snapshots during 1 ps of MD). Left: in water (x = 8); right: in acetonitrile (x = 9).

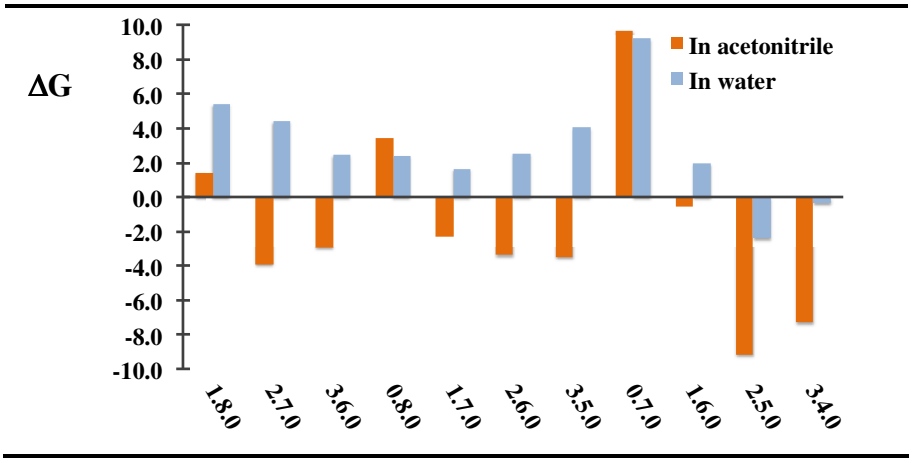


Figure S6: Speciation histogram from "**0.9.0** + 3 Cl^-" in acetonitrile (*orange*) and in water (*blue*). Free energies are in kcal/mol. Values are given in Table S8

Full citation for Gaussian 03:

Gaussian 03, Revision E.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, Gaussian, Inc., Pittsburgh, PA, 2003

Full citation for Gaussian 09:

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Revision A.02, Gaussian, Inc., Wallingford CT, 2009.

Cartesian Coordinates in xyz format (BLYP/SDD optimized)

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----------------------------------------
   28
0.9.0
La    -0.000361    -0.001511     0.000691
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 O     0.007594    -0.579370     2.570949
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 O    -1.845151     1.355246     1.260644
 O     0.012379     2.517444    -0.773334
 O     1.843032    -1.773844     0.527197
 O    -1.861334    -1.749131     0.544143
 O    -0.019039    -1.914309    -1.812987
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 H     1.918007     1.196911    -2.362134
 H     2.699890     1.720869     0.885875
 H     1.933219     1.430812     2.212832
 H    -0.518082    -0.140596     3.271404
 H     0.522971    -1.277316     3.025713
 H    -2.690603     0.955085    -1.702781
 H    -1.930225    -0.036648    -2.636024
 H    -2.667427     1.040853     1.690540
 H    -1.891076     2.333285     1.292498
 H    -0.518277     2.918479    -1.492404
 H     0.547699     3.248248    -0.400634
 H     2.662345    -1.681818     1.056353
 H     1.888192    -2.667743     0.128975
 H    -1.914998    -2.270175     1.371974
 H    -2.681816    -1.956832     0.050765
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 H    -0.543297    -2.741749    -1.804132

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 C     3.762079     1.022070    -3.638454
 H     4.373617     1.882627    -3.324668
 H     3.290964     1.254869    -4.606525
 H     4.419385     0.147386    -3.764435
 N     1.979483    -1.764429     0.510066
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 H     3.455451    -4.494823     1.217117
 H     4.472882    -3.184427     1.892686
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 H    -3.235010    -4.645237     1.266832
 H    -4.358583    -3.834548     0.131313
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 H     1.117308    -3.924189    -4.139479
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 H    -0.181361    -4.799997    -3.271745
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 C     0.029451    -0.965526     3.755633
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 H    -0.760230    -0.802157     5.708420
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 N    -0.068700     2.606029    -0.730914
 C    -0.100134     3.733176    -1.044243
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 H    -0.002491     5.784747    -0.550936

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 H    -0.667844    -2.873996    -1.546554
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 H     2.200209    -2.328520     1.478989
 H    -0.561795     1.013058    -3.204297
 H    -1.775681     0.582542    -2.292121
 H     0.977580     2.945977    -0.681456
 H     2.190063     2.338685    -1.479309
 H    -0.557949    -1.018181     3.202769
 H    -1.773053    -0.587709     2.292298
 H    -0.678071     2.871092     1.547667
 H    -1.750051     2.342296     0.543477
 O     1.966676     0.867731     1.631850
 H     2.201359     0.875822     2.579784
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Cl    -2.639320    -0.926208    -0.358602
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 C     2.219843     1.172874     2.904468
 C     3.052341     1.605994     4.028236
 H     2.730969     2.599725     4.376609
 H     2.963076     0.892335     4.861837
 H     4.108120     1.662406     3.721601
 C    -0.014472    -2.234572    -3.236093
 C    -0.213148    -3.095567    -4.402141
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 O   -1.763653     1.534092     1.330417
Cl    0.019627     2.683083    -0.925744
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 O   -2.078603    -1.523549     0.882380
Cl   -0.039437    -2.472469    -1.252637
 H    1.719054    -0.515524    -2.485040
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 H   -1.781414    -0.476040    -2.450032
 H   -1.889418     1.728947     2.278529
 H   -1.600776     2.393957     0.876865
 H    2.967892    -1.258855     0.632936
 H    1.870698    -2.302918     0.208182
 H   -1.914666    -2.262110     0.247702
 H   -2.980163    -1.194836     0.694535
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Cl    0.645740     0.571788    -2.696424
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Cl   -0.042968    -2.840125     0.002661
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 H    1.377969    -3.831867     2.474799
 H    2.909681    -3.363519     3.295249
 C    2.760607     2.777928    -0.126546
 C    3.792650     3.775788    -0.413393
 H    3.482450     4.765884    -0.045821
 H    4.738375     3.496974     0.076128
 H    3.958021     3.836120    -1.500286
 C   -2.688646    -1.462139    -2.516103
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 H   -3.227614    -3.268041    -3.459374
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Cl    0.004674    -0.666177     2.878801
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Cl    0.013492     2.827679    -0.851366
 O    1.802380    -1.824750     0.544425
 O   -1.819858    -1.803405     0.556911
Cl   -0.018133    -2.149344    -2.029980
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 H    1.598345     1.309341    -2.181715
 H    1.613551     2.296212     1.059360
 H    1.611912     1.211163     2.224893
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 H   -1.598291    -0.225788    -2.522022
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 H   -1.579955     2.314710     1.069768
 H    1.578601    -2.097144     1.460997
 H    1.573938    -2.561861    -0.062586
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Cl   -0.012619    -0.614616     2.730224
 N   -2.175490     0.430340    -1.775095
 N   -2.156362     1.366255     1.239266
Cl    0.034001     2.669565    -0.837462
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 N   -2.185240    -1.728210     0.537275
Cl   -0.021402    -2.042466    -1.912078
 C    3.617786    -3.861538     1.178406
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 H    3.417567    -4.157320     2.220013
 H    3.370677    -4.705541     0.515740
 H    4.690353    -3.634797     1.075737
 C    2.855901     2.013061     1.900986
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 H     3.154777    -0.736730     0.243512
 H     3.116343     0.108974    -1.065402
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 O    -0.628650     0.656740     2.417965
 H    -1.327558     0.292054     3.002057
 H    -0.229793     1.396047     2.924705
 O    -2.005095     1.567044    -0.444924
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 O    -2.166029    -1.372957     0.309818
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 O     0.086368    -1.999425    -1.633564
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 N     2.566189    -0.425401    -0.566048
 C     3.696238    -0.603469    -0.817613
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 H     5.551149     0.099743    -1.534630
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 C    -0.105358    -3.582436    -1.360221
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 H     2.785040     0.371010    -1.017187
 O     0.953584     2.272514     0.891971
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 H    -1.057890     0.454038     3.333785
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 O    -2.357205    -1.238808     0.498248
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 O     0.159146    -2.166215    -1.405006
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Cl     0.443251     0.805003    -2.353194

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 H     5.567424     0.364428    -1.108552
 H     5.335417    -0.990126    -2.259165
 N    -1.418191     1.155771     2.017166
 C    -1.925391     1.780690     2.865805
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 H    -1.931113     3.455660     4.143649
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Cl     0.507192     0.760686    -2.543264

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Cl     6.307986     3.396337     1.547129
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 C     1.216812     4.530229     5.084465
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 O    -1.748266     1.854152    -0.240856
 H    -2.394633     2.181115     0.423955
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 O     0.709218    -2.393599    -0.972812
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