Why Are Saccharides Dehydrated in the Presence of Electrolytes? Insights from Molecular Modeling and Thermodynamic Measurements

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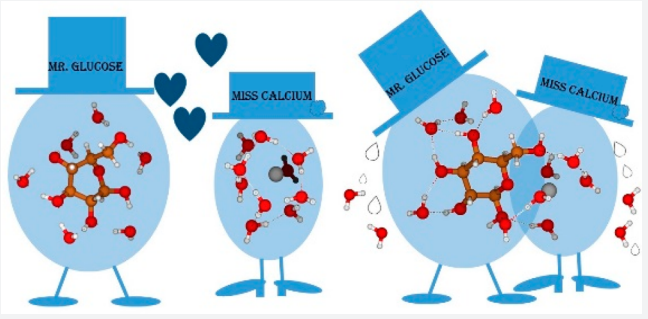
Supporting Information

ABSTRACT: The mechanisms governing the interactions of neutral polar solutes with ions in aqueous solutions are still poorly understood, despite the importance of this phenomenon in many fields (chemistry, physicochemistry, biology, food industries). In order to go further through the understanding of the molecular mechanisms governing the ions' specific effects, this paper presents a generic method dealing with the characterization and understanding of interactions between saccharides and ions in aqueous systems. For that, an original approach combining a computational technique and experimental measurements (thermodynamic properties) is proposed to explain and rationalize the relationship between the solute hydration and the physical chemistry of the ions in solution (cation/anion, charge, size, and hydration). These relationships make it possible to evaluate the hydration state of a saccharide, a polar neutral molecule, according to the ionic composition, from the knowledge of the ions' hydration properties. This work proposes new insight into molecular mechanisms governing the polar neutral solute/ion interactions and a new understanding of the hydration phenomenon in electrolytic solutions.



More than a century ago, Hofmeister found a particular ordering of ions in the ability of salts to precipitate egg white.[1] His main conclusion was that the salts' effectiveness in precipitating proteins is related to the ions' capacity to order water. Today this phenomenon refers to hydration. An important point that he highlights is that ions cannot be considered as isolated species in water. The salting-out effect is a ubiquitous phenomenon in chemistry, biochemistry, biophysics, and food.[2] Despite the understanding of a crucial specific effect of ions in the development of such areas, the influence of cations and anions on polar neutral solutes is still poorly understood.

In order to contribute to the understanding of the molecular level mechanisms governing the ions' specific effects on biocompounds, this paper deals with the characterization and the understanding of interactions between saccharides and electrolytes. Indeed, studies of the interactions between saccharides and electrolytes have been attracting renewed interest over the last 20 years.[3−9]

Up to now, the influence of the electrolyte on the saccharide hydration state has been interpreted using the structural hydration model,[10] based on the cosphere concept developed by Gurney.[11] According to this model, the influence of the solute on the structure of water is the solute is represented by a shell of water surrounding the solute. The overlap of the hydration cosphere of the saccharide and of the ions (saccharide/ion interactions) then leads to the saccharide dehydration. More recently, the influence of the electrolyte on the saccharide hydration has been characterized by the molar volume. The study has highlighted that the dehydration mechanism results from multiple interactions taking place at the molecular scale (saccharide/ions; ions/water).[12] Therefore, the link between the saccharide hydration state and the ions' properties (cation/anion, charge, size, and hydration) needs to be deepened.

Effects observed at the macroscopic scale, such as changes in apparent molar volume, result from nanoscale phenomena. Thus, it is necessary to develop new complementary approaches to characterize the systems at the microscopic scale. Molecular modeling, and more precisely quantum mechanics, are particularly adapted for describing systems at this scale.

In this context, the objective of this work is to go further through the understanding of the mechanisms that govern polar neutral solutes hydration as a function of the ionic composition. The original methodology envisaged is based on experimental and theoretical approaches at different scales. The fundamental approach proposed consists, on the one hand, of characterizing the hydration properties of the ions by using quantum mechanics. On the other hand, it relies on the study of the relationship between the hydration properties of saccharides,

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based on experimental measurements, and the ion properties obtained.

In our previous work, a systematic volumetric study of saccharides (xylose, glucose, and sucrose) in the presence of various electrolytes (LiCl, NaCl, KCl, Na_2SO_4, K_2SO_4, $CaCl_2$, $MgCl_2$, $MgSO_4$) has been carried out from density measurements at 298.15 K.[12] From this data, the saccharide hydration number at infinite dilution n_H (expressed in molecules of water per molecule of solute), which explicitly reveals the solute hydration degree, has been calculated for different ionic compositions. The results are given in Supporting Information, in Table S1. First of all, for an infinite dilution in water, saccharide hydration numbers are 3.9, 4.7, and 7.9 for the xylose, glucose, and sucrose respectively (Table S1). These values match the number of hydroxyl groups present in each saccharide (4, 5, and 8 for the xylose, glucose, and sucrose respectively). On the other hand, for an infinite dilution in the various electrolytes, the saccharide hydration number decreases with the increase of the electrolyte molality (for instance, see sucrose in Figures S1 and S2 in Supporting Information). This phenomenon depends on the electrolyte nature. With regard to the impact of the cation, the saccharides dehydration increases according to the following sequence (Figure S1):

$$Li^+ < Na^+ < K^+ < Mg^{2+} < Ca^{2+}$$

Concerning the impact of the anion, the saccharides dehydration increases according to the following sequence (Figure S2):

$$Cl^- < SO_4^{2-}$$

Whatever the ion (cation or anion), saccharides are further dehydrated in the presence of divalent ions than in the presence of monovalent ones. That can be attributed to stronger attractive electrostatic interactions between the hydrophilic groups of the saccharides and the divalent ions. These interactions govern the dehydration phenomenon. Moreover, for a given ion valence, previous work has highlighted that saccharides dehydration increases with the decrease of the ion free energy of hydration, i.e., lower ion−water interactions. Thus, ion−water interactions have to be considered for a better understanding of the saccharide hydration properties in the presence of various ions.[12]

Ions hydration properties were carried out at the density functional theory (DFT) level of theory, the B3PW91 functional[13] and 6-31++G** basis sets with the Gaussian 09 suite of programs (see Supporting Information). The water-shell around the solutes is obtained using the methodology proposed by Castro et al.[14] for mercury compounds and also by Zhao et al.[15] for samarium complexes. In summary, the solvation shell is constructed in a stepwise manner by adding one water molecule at a time. At each step, a full geometry optimization of the system is performed without any symmetry constraints. The coordinates of the optimized hydrated structures and figures showing the spatial water molecules arrangement are provided in Supporting Information.

The solvation enthalpy of the ion ΔH_w is calculated as the difference between the enthalpy of the complex ($H_{complex}$) and those of the two separated fragments, namely, the ion (H_{ion}) and the water cluster ($H_{hyd.shell}$).

$$\Delta H_W = H_{complex} - H_{ion} - H_{hyd.shell} \quad (1)$$

The ion first-hydration shell is considered to be complete when the interaction energy between the ion and the water reaches a plateau, i.e., is stable with respect to water addition, as defined by eq 1. On these structures, the ion coordination number is thus defined as the number of water molecules directly bonded to the central ion in its first layer of solvation sphere. In the following, a water molecule is considered in direct interaction with the ion, if the bond length is shorter than the sum of the van der Waals radii of the atom in interaction.[16] In addition, in the case of anions, hydrogen bonds have to be established between the hydrogen of the water molecule and the anion.

The structural parameters of the ions hydration shell, i.e., the ion coordination number, its optimized coordinated water structure, and the average distance between the ion and the water molecules, are listed in Table 1. For comparison, other results from molecular modeling are also reported.[17−26] One can state that our values are consistent with the literature, indicating the validity of our approach and assumptions.

Concerning the cation, the number of water molecules belonging to the first solvation shell depends on the nature of the cation. The optimized building blocks, corresponding to the first observed plateau of the $\Delta H_w = f$ (water number) curve for the different cations, reveal that 4, 5, 6, 6, and 8 water molecules are respectively involved in the first hydration sphere of Li^+, Na^+, K^+, Ca^{2+}, and Mg^{2+} (Table 1). Interestingly, the coordination number of the monovalent cations can be ranked according to the sequence: $Li^+ < Na^+ < K^+$ and for the divalent cations: $Mg^{2+} < Ca^{2+}$. For a monovalent cation, the K^+ coordination number is larger than those of Li^+ and Na^+, as expected from the larger size of K^+ compared to Li^+ and Na^+. Indeed, because of steric hindrance, smaller ions, such as Li^+ for monovalent cations (Mg^{2+} for divalent cations), have fewer coordinated water molecules than other ions of identical valence. Moreover, the shorter M^+−water distance is found for Li^+. This shorter distance is associated with the radial expansion of the valence orbital of the cation and indicates that the cation−water interaction involves atomic orbital overlap contributions. Therefore, the shortest is the distance, the largest is the overlap, and as a result, the strongest is the water−cation interaction. Likewise, both the coordination number and the cation−water distance of Mg^{2+} are lower than those of Ca^{2+}. Comparing monovalent and divalent cations having the same coordination number, for instance, K^+ and Mg^{2+}, the Mg^{2+}−water distance is shorter than the K^+−water one. This is again associated with the lowest radial expansion of the orbital of divalent metals with respect to monovalent ones. Using the same argument as before, this means that the cation−water interactions are stronger with Mg^{2+} than with K^+.

Concerning the anion hydration properties, the coordination numbers of Cl^- and SO_4^{2-} are respectively 5 and 9. The sulfate anion, which is a polyatomic molecule, is a highly hydrated anion, with a very compact water shell, compared to Cl^-. Unlike the water−cation interactions where bonding is essentially due to orbital overlap, the water−anion interactions are mainly hydrogen bonds. For monatomic anions such as Cl^-, that leads to a competition between the water network formation and the solvation of the anion. The consequence of this competition is that the structure of the water network around Cl^- is relaxed.

To evaluate the role of the electrolyte on the saccharide hydration state, the influence of the cations and anions will be first quantified separately.

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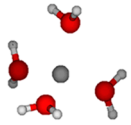
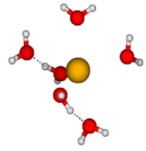
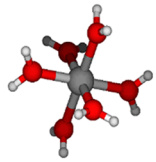
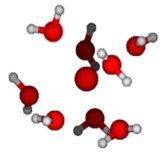
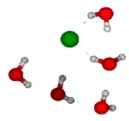
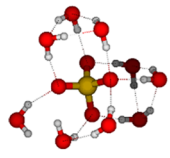
Table 1. Structural Parameters of the Ion Hydration Shell[a]

	Li^+	Na^+	K^+
CN	4	5	6
	4[17-19]	5.2[20], 5.85[17]	6[22]
		5-6[21]	6.1-6.7[20]
Optimized structure			
d (Å)	1.99-2.11	2.36-2.53	2.81-2.92
		2.3-2.5[20]	2.75-2.80[20]
		2.40[21]	

	Mg^{2+}	Ca^{2+}
CN	6	8
	6[23-24]	5-8[23], 6[24]
	5-6[21]	8[25],7-8[21]
Optimized structure		
d (Å)	1.95-2.12	2.42-2.52
	2.13[23]	2.42-2.58[23]
	2.09[21]	2.52[21]

	Cl^-	SO_4^{2-}
CN	5	9
	6.25[17]	10-11[21]
	≥5-6[21]	
Optimized structure		
d (Å)	2.30-2.49	1.81-1.91
	2.24-2.42[26]	1.91[21]
	2.37[21]	

[a]Values obtained in the present work are reported in the first row of the table. CN: coordination number, optimized structure: water cluster coordinated to the ion, *d*: average distance between ion and coordinated water molecules.

Considering first the effect of the cation, the possible existence of correlations between the cation coordination number and the saccharide hydration number in electrolyte solutions was investigated. The experimental saccharide hydration numbers, calculated for different electrolytes containing either Cl^- or SO_4^{2-} and for a given cation molality (1 mol·kg^{-1}), are represented as a function of the computed coordination number of the cations (Figure 1). The saccharides are all the more

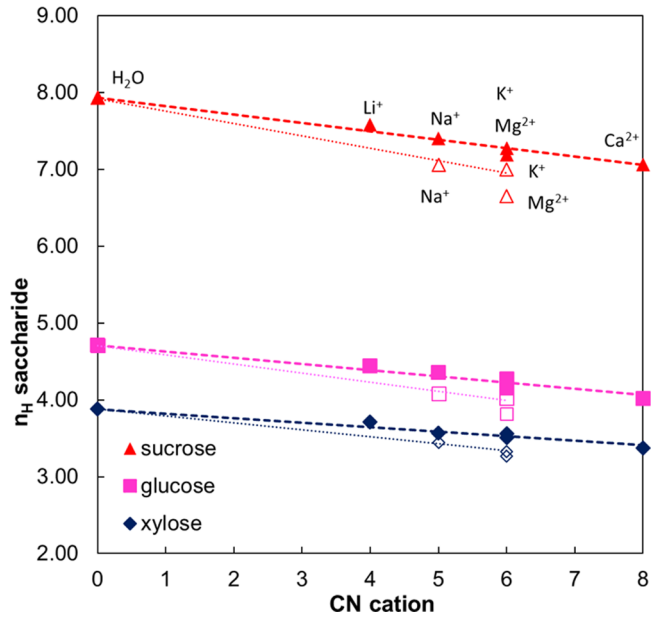


Figure 1. Saccharide hydration numbers (n_H saccharide) versus the coordination numbers (CN cation) of different electrolytes containing Cl^- (filled symbols) and SO_4^{2-} (empty symbols) for a given cation molality (1 mol·kg^{-1}).

dehydrated as the cations coordination number (i.e., the number of water molecules directly interacting with the cation) increases (Figure 1). The large saccharide dehydration observed in the presence of divalent ions can be attributed to the lowest radial expansion of the orbital of divalent metals with respect to monovalent ones, as previously mentioned. This means that the interactions between cations and the oxygen of the saccharide hydroxyl groups are stronger with divalent cations than with monovalent ones. As a consequence, saccharides are more dehydrated. Moreover, focusing on the electrolyte bearing a Cl^- counteranion, the saccharide hydration number decreases linearly with the increase of the cation coordination number (linear regression coefficient >0.95 for the three saccharides). The existence of this linear relation indicates that the presence of Cl^- has a weak impact on the saccharide hydration. This is further highlighted by the extrapolation of the saccharide coordination number from this linear relationship. Indeed, it is noteworthy that the saccharide hydration numbers, obtained by extrapolation of the straight line to CN = 0, which represents the hydration state of each saccharide in pure water, are very close to the values determined from the saccharide apparent molar volumes. For instance, the glucose hydration number, obtained by extrapolation is 4.75 (electrolyte at 0.15 mol·kg^{-1}), compared to the value obtained from the saccharide apparent molar volumes which is 4.72. Furthermore, the saccharide hydration numbers, for cations having the same coordination number (K^+ and Mg^{2+}), are close. For example, the hydration number of xylose with KCl is 3.56, which is very close to the value of 3.51

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determined in the presence of $MgCl_2$. A stronger difference between the sucrose hydration number in the presence of KCl (n_H = 7.27) and of $MgCl_2$ (n_H = 7.19) is, however, observable. Indeed, sucrose is more sensitive to the dehydration caused by the presence of the divalent cations because of its large number of hydroxyl groups. Besides, the saccharide dehydration increases with the number of hydrophilic groups contained in each saccharide. Indeed, the straight slopes for xylose, glucose, and sucrose are −0.08, −0.11, and −0.13, respectively (Figure 1).

Hence, in the presence of Cl^-, the fact that the saccharides are all the more dehydrated than the cation coordination number is important (i.e., increase of the number of water molecules contained in the first coordination shell of the cation). That means that the greater the cation coordination number is, the more it can create interactions with the saccharide. The saccharide−water interactions that hydrated the hydrophilic groups of the saccharides are then replaced by saccharide−cation interactions. Equally, the cation−water interactions are replaced by cation-hydrophilic group interactions. Both saccharide and cation are dehydrated. It appears that the anion Cl^- has a weak impact on the saccharide hydration. In the presence of the chloride anion, interactions in solution are then governed by the cation−saccharide interactions. To our best knowledge, such a conclusion has never been reported to date.

In a second step, the anion influence was studied. Figure 1 shows that the saccharide dehydration effect is much larger with electrolyte containing the sulfate ion than the chloride anion. The sulfate anion promotes saccharide dehydration. On the one hand, the larger influence of the sulfate ion is linked to its higher charge (divalent anion) that creates more hydrogen bonds with the saccharides. On the other hand, it can be correlated with its greater coordination number (9) compared to the chloride ion (5) and the shorter anion−water distance (Table 1). For sulfate electrolytes with monovalent cations (Na^+ and K^+), the saccharide hydration number also decreases linearly with the increase of the coordination numbers of the cations. Furthermore, the divalent cations remain the most dehydrating component compared to monovalent cation. However, for cations having the same coordination number (K^+ and Mg^{2+}), unlike the results obtained in the presence of Cl^-, the saccharide hydration numbers are different. Indeed, the sucrose hydration number is 7.00 in the presence of K_2SO_4 and 6.65 in the presence of $MgSO_4$. That shows the strong impact of the sulfate anion on the saccharide hydration. Hence, in order to evaluate possible synergistic effects of anion and cation on the saccharide hydration, the possible existence of a correlation between the saccharide hydration numbers (n_H) and the total coordination numbers of the ions of the electrolyte (CN_{total} = CN_{cation} + CN_{anion}) is studied (Figure 2). The CN_{total} takes into account the stoichiometric coefficients of the electrolyte ions. For example, the CN_{tot} of Na_2SO_4 is twice the CN of Na^+ to which the CN of SO_4^{2-} is added (see Table 1), meaning a total coordination number (CN_{total}) of 19.

In the presence of SO_4^{2-}, the saccharides hydration numbers decrease linearly with the increase of the total coordination number of the ions (linear regression coefficients > 0.94). This is indicative of the effect of SO_4^{2-} on the saccharide dehydration. As in the presence of Cl^-, the saccharide dehydration increases with the saccharides' hydrophilic groups number, which is consistent. Indeed, the straight slopes for xylose, glucose, and sucrose are −0.02, −0.03, and −0.05, respectively.

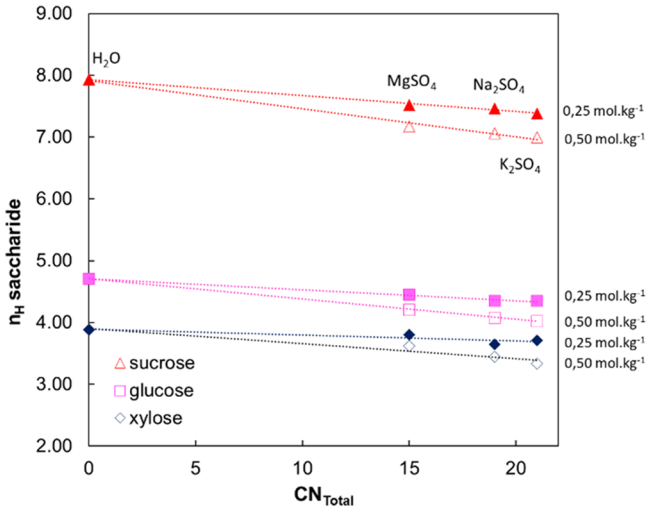

Figure 2. Saccharide hydration numbers (n_H saccharide) versus the total coordination numbers of electrolytes (CN_{total}) containing SO_4^{2-} for different electrolyte molalities (0.25 and 0.5 mol·kg^{-1}).

Finally, in order to take into account the influence of the electrolyte concentration and since it was demonstrated that Cl^- exhibits a weak influence on the dehydration, a generalized coordination number is defined by including the molality of ions in electrolyte as follows:

$$\overline{CN_{total}} = CN_{cation} \cdot m_{cation} \quad \text{for chloride electrolytes} \tag{2}$$

$$\overline{CN_{total}} = CN_{anion} \cdot m_{anion} + CN_{cation} \cdot m_{cation} \quad \text{for sulfate electrolytes} \tag{3}$$

with CN_{cation} or CN_{anion}: cation or anion coordination numbers, respectively, and m_{cation} or m_{anion}: cation or anion molality (mol·kg^{-1}).

The evolution of the saccharide hydration number in sulfate electrolytes, for various ionic composition, is represented in Figure 3 as a function of $\overline{CN_{total}}$. The one concerning Cl^- is presented in Figure S3.

For each saccharide and regardless of the electrolyte concentration, saccharide hydration numbers decrease linearly with $\overline{CN_{total}}$, which is remarkable. The total cation coordination number reflects then the ions' ability to form direct interactions with the saccharide hydroxyl groups. It takes into account the proportions of the cations and anions of the solution and the number of opportunities for ions to interact with saccharides.

Moreover, the relationships established enable the determination of the saccharide hydration numbers from the knowledge of the ions properties.

This work constitutes a new approach, which allows the understanding of mechanisms governing the ions' specific effects on polar neutral molecules. More precisely, it deals with phenomena governing saccharide hydration, as a function of the physical chemistry properties of ions in solution (cation or anion charge, size, and hydration). To this end, an original methodology based on the combination of experimental measurements (molar volume) and computational technique has been used.

From experimental data, the saccharide hydration number has been calculated in various electrolytes, for different ionic compositions. Ions hydration properties were computed using

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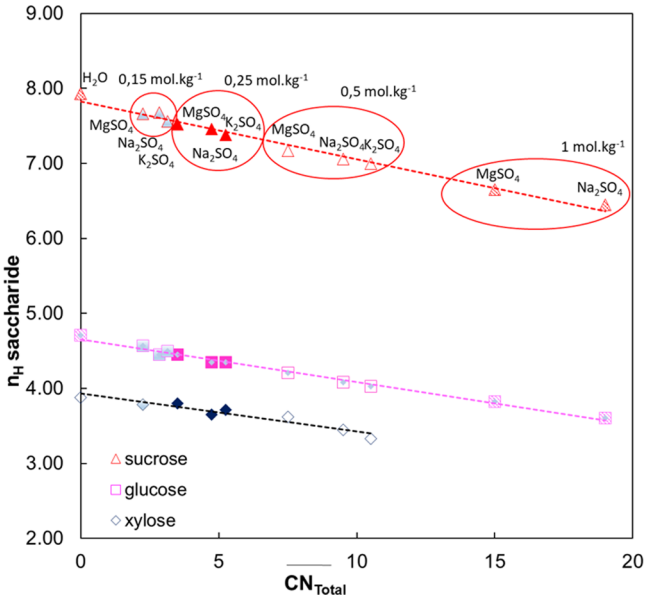

Figure 3. Saccharide hydration numbers (n_H saccharide) versus the total coordination numbers of electrolytes containing SO_4^{2-} (CN_{total}) for different electrolyte molalities (0.25, 0.5, 1 mol·kg^{-1}).

theoretical methods (DFT). Saccharide and ions properties obtained from these two complementary methods were then put in parallel, in order to rationalize the relation between the saccharide hydration number in electrolyte solution and the hydration properties of ions.

The influence of the cations and anions on the saccharide hydration has been quantified separately.

The study of the influence of cations highlights that saccharide dehydration increases with the increase of the cation coordination number (i.e., the number of water molecules directly interacting with the cation), whatever the cation valence. Divalent cations have a larger impact on the saccharide dehydration than monovalent ones. That can be attributed to the lowest radial expansion of the orbital of divalent metal with respect to monovalent ones. Interactions between cations and the oxygen of the saccharide hydroxyl groups (the cation−oxygen interaction involving in atomic orbital overlap) are therefore stronger with divalent cations than with monovalent ones. This causes higher saccharide dehydration. For a given cation valence, the cation coordination number increases with the size of the cation. That allows the cation to create more saccharide−cation interactions and then to further dehydrate the saccharide. The cation coordination number reflects the ions' ability to form direct interactions with the saccharide hydroxyl groups.

Concerning the influence of the anion on the saccharide hydration, this work has highlighted that Cl^- has weak interactions with saccharides. Then, the saccharide hydration number only depends on the cation coordination number. In sharp contrast, SO_4^{2-} has strong interactions with saccharides. In this case, the saccharide hydration number depends on the coordination number of both cations and of anions of the electrolyte.

Relationships established in this work make possible to evaluate the hydration state of a polar neutral solute, a saccharide, as a function of the ionic composition, from the knowledge of the ions' hydration properties.

The results of the scaling up may be transferable to other polar and neutral biomolecules. It would be interesting to study what would become of the relationships obtained with molecules having a charged or hydrophobic part.

METHODS

Apparent molar volumes of saccharides, $V_{\Phi,S}$, which characterize the hydration state of the solute, have been determined in ref 12. At infinite dilution, the apparent molar volumes, $V^0_{\phi,S}$, are equal in value to the standard partial molar volumes. The partial molar volume of a nonelectrolyte can be divided in two terms: the intrinsic molar volume of the nonhydrated solute, V_{int}, and the electrostriction partial molar volume, V_{elect}, due to the interaction of the nonelectrolyte with water (shrinkage in volume):[27]

$$V^\circ_{\Phi S} = V_{int} + V_{elec} \tag{4}$$

The positive intrinsic volume is given by the size of the solute molecule, and for a given temperature, it is considered that it remains at the same magnitude in water and aqueous salt solutions. The interaction term V_{elect} is variable and depends on the interactions between the solute molecule and surrounding the water molecules (hydration shell).

The hydration number n_H (or solvation number, expressed in molecules of water per molecule of solute) explicitly reveals the hydration degree of a solute in water. The hydration number can be calculated from the volumetric properties using the following equation:[28,29]

$$n_H = \frac{(V^0_e - V^0_b)}{V_{elec}} \tag{5}$$

where V^0_e is the molar volume of electrostricted water, and V^0_b is the molar volume of bulk water. The value of $(V^0_e - V^0_b)$ is about −3.3 cm^3·mol^{-1} at 298.15 K.[28,29] The V_{elec} values can be obtained from rearrangement of eq 4 as follows:

$$V_{elec} = V^0_{\Phi S} - V_{int} \tag{6}$$

The intrinsic volume V_{int} for saccharides is calculated from the crystal molar volume (eq 7).

$$V_{int} = \left(\frac{0.7}{0.634}\right)\frac{M}{d_{cryst}} \tag{7}$$

where M is the molar mass of saccharide, 0.7 is the packing density for molecules in organic crystals, and 0.634 is the packing density for random packed spheres. The crystal density (d_{cryst}) determined by single-crystal X-ray diffraction is 1.52 g·cm^{-3} for the xylose,[30] 1.56 g·cm^{-3} for the glucose,[31] and 1.59 g·cm^{-3} for the sucrose.[32] The obtained n_H values are reported in Table S1 (Supporting Information).

Safety. No unexpected or unusually high safety hazards were encountered.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acscentsci.8b00610.

Supplementary figures; tabulated values of saccharides hydration numbers at infinite dilution; Gaussian full references; computational details;[13,33,34] electronic energies, enthalpies, and Cartesian coordinates of the

stationary points on the potential energy surfaces and optimized water structure surrounding ions (PDF)

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Notes

The authors declare no competing financial interest.

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REFERENCES

(1) Vlachy, N.; Jagoda-Cwiklik, B.; Vácha, R.; Touraud, D.; Jungwirth, P.; Kunz, W. Hofmeister series and specific interactions of charged headgroups with aqueous ions. *Adv. Colloid Interface Sci.* **2009**, *146* (1−2), 42−47.

(2) Kunz, W. Specific ion effects in colloidal and biological systems. *Curr. Opin. Colloid Interface Sci.* **2010**, *15* (1−2), 34−39.

(3) Zhuo, K.; Wang, J.; Yue, Y.; Wang, H. Volumetric properties for the monosaccharide (D -xylose, D -arabinose, D -glucose, D -galactose) − NaCl − water systems at 298.15 K. *Carbohydr. Res.* **2000**, *328*, 383−391.

(4) Seuvre, A. M.; Mathlouthi, M. Solutions properties and solute-solvent interactions in ternary sugar-salt-water solutions. *Food Chem.* **2010**, *122*, 455−461.

(5) Parke, S. A.; Birch, G. G.; Dijk, R. Some taste molecules and their solution properties. *Chem. Senses* **1999**, *24*, 271−279.

(6) Warmińska, D. Volumetric and acoustic properties of D-mannitol in aqueous sodium or magnesium chloride solutions over temperature range of 293.15−313.15 K. *Carbohydr. Res.* **2012**, *349*, 44−51.

(7) Banipal, P. K.; Singh, V.; Aggarwal, N.; Banipal, T. S. Hydration behaviour of some mono-, di-, and tri-saccharides in aqueous: Volumetric and rheological approach. *Food Chem.* **2015**, *168*, 142−150.

(8) Thirumaran, S.; George, G.; Bakkiyalakshmi, P. Acoustical Behaviour of Disaccharide (Sucrose) in Aqueous Alkali Metal Halides at Varying Temperatures. *Chem. Sci. Trans.* **2014**, *3* (1), 323−331.

(9) Palani, R.; Kalavathy, S. Volumetric compressibility and transport studies on molecular interactions of mono, di and tri saccharides in aqueous sodium butyrate mixtures at 303.15 K. *Pelagia Res. Libr.* **2011**, *2*, 146−155.

(10) Desnoyers, J. E.; Arel, M.; Perron, G.; Jolicoeur, C. *J. Phys. Chem.* **1969**, *73* (11), 3346−3351.

(11) Gurney, R. W. *Ionic Proccesses in Solution*; McGraw-Hill Book Company: New York, 1953.

(12) Teychene, J.; Roux-de Balmann, H.; Galier, S. Role of the triple Solute/Ion/Water interactions on the saccharide hydration: a volumetric approach. *Carbohydr. Res.* **2017**, *448*, 118−127.

(13) Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993**, *98* (7), 5648−5652.

(14) Castro, L.; Dommergue, A.; Renard, A.; Ferrari, C.; Ramírez-Solís, A.; Maron, L. Theoretical study of the solvation of $HgCl_2$, $HgClOH$, $Hg(OH)_2$ and $HgCl_3$: A density functional theory cluster approach. *Phys. Chem. Chem. Phys.* **2011**, *13* (37), 16772−16779.

(15) Zhao, X.; Perrin, L.; Procter, D.; Maron, L. The role of H_2O in the electron transfer−activation of substrates using SmI2: Insights from DFT. *Dalton Transactions* **2016**, *45*, 3706−3710.

(16) Batsanov, S. S. Van der Waals Radii of Elements. *Inorg. Mater.* **2001**, *37* (9), 871−885.

(17) Ohrn, A.; Karlstrom, G. A. Combined Quantum Chemical Statistical Mechanical Simulation of the Hydration of Li^+, Na^+, F^- and Cl^-. *J. Phys. Chem. B* **2004**, *108*, 8452−8459.

(18) Loeffler, H. H.; Rode, B. M. The hydration structure of the lithium ion. *J. Chem. Phys.* **2002**, *117*, 110−117.

(19) Rempe, B. S.; Pratt, L. R.; Hummer, G.; Kress, J. D.; Martin, R. L.; Redondo, R. The Hydration Number of Li^+ in Liquid Water. *J. Am. Chem. Soc.* **2000**, *122*, 966−967.

(20) Bankura, A.; Carnevale, V.; Klein, M. L. Hydration structure of salt solutions from ab initio molecular dynamics. *J. Chem. Phys.* **2013**, *138*, 014501.

(21) Fuoco, A.; Galier, S.; Roux-de Balmann, H.; De Luca, G. Correlation between Computed Ion Hydration Properties and Experimental Values of Sugar Transfer through Nanofiltration and Ion Exchange Membranes in Presence of Electrolyte. *Computation* **2018**, *6* (42), 1−11.

(22) Varma, S.; Rempe, S. B. Coordination numbers of alkali metal ions in aqueous solutions. *Biophys. Chem.* **2006**, *124*, 192−199.

(23) Ikeda, T.; Boero, M.; Terakura, K. Hydration properties of magnesium and calcium ions from constrained first principles molecular dynamics. *J. Chem. Phys.* **2007**, *127*, 074503.

(24) León-Pimentel, C. I.; Amaro-Estrada, J. I.; Hernández-Cobos, J.; Saint-Martin, H.; Ramírez-Solís, A. Aqueous solvation of Mg(II) and Ca(II): A Born-Oppenheimer molecular dynamics study of micro-hydrated gas phase clusters. *J. Chem. Phys.* **2018**, *148* (14), 144307.

(25) Schwenk, C. F.; Loeffler, H. H.; Rode, B. M. Molecular dynamics simulations of Ca^{2+} in water: Comparison of a classical simulation including three-body corrections and Born − Oppenheimer ab initio and density functional theory quantum mechanical/molecular mechanics simulations. *J. Chem. Phys.* **2001**, *115*, 10808.

(26) Tongraar, A.; Rode, B. M. Ab initio QM/MM dynamics of anion−water hydrogen bonds in aqueous solution. *Chem. Phys. Lett.* **2005**, *403*, 314−319.

(27) Friedman, H. L.; Krishnan, C. V. Studies of hydrophobic bonding in aqueous alcohols: Enthalpy measurements and model calculations. *J. Solution Chem.* **1973**, *2* (2), 119−140.

(28) Shekaari, H.; Kazempour, A. Dehydration effect of ionic liquid, 1-pentyl-3-methylimidazolium bromide, on the aqueous d-glucose solutions: Thermodynamic study. *J. Taiwan Inst. Chem. Eng.* **2012**, *43* (4), 650−657.

(29) Millero, J. F.; Lo Surdo, A.; Shin, C. The Apparent Molal Volumes and Adiabatic Compressibilities. *J. Phys. Chem.* **1978**, *82* (7), 784−792.

(30) Weast, C. *Handbook of Chemistry and Physics*, 68th ed.; CRC Press, 1987.

(31) McDonald, T. R.; Beevers, C. The crystal and molecular structure of α-glucose. *Acta Crystallogr.* **1952**, *5*, 654−659.

(32) Charalambous, G. *Handbook of Food and Beverage Stability: Chemical, Biochemical, Microbiological, and Nutritional Aspects*; Academic Press: Orlando, 1986.

(33) Ditchfield, R.; Hehre, W. J.; Pople, J. A. Self-Consistent Molecular-Orbital Methods. IX. An Extended Gaussian-Type Basis for Molecular-Orbital Studies of Organic Molecules. *J. Chem. Phys.* **1971**, *54*, 724−728.

(34) Frisch, M. J.; Pople, J. A.; Binkley, J. S. Self-Consistent Molecular Orbital Methods. 25. Supplementary Functions for Gaussian Basis Sets. *J. Chem. Phys.* **1984**, *80*, 3265−3269.

Supporting information for:

Why saccharides are dehydrated in presence of electrolyte? Insights from molecular modeling and thermodynamic measurements.

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Figures

Figure S_1: Sucrose hydration number (n_H) versus the cation molality (m_{cation}) for electrolytes containing Cl^- (figure S1-a) and SO_4^{2-} (Figure S1-b).

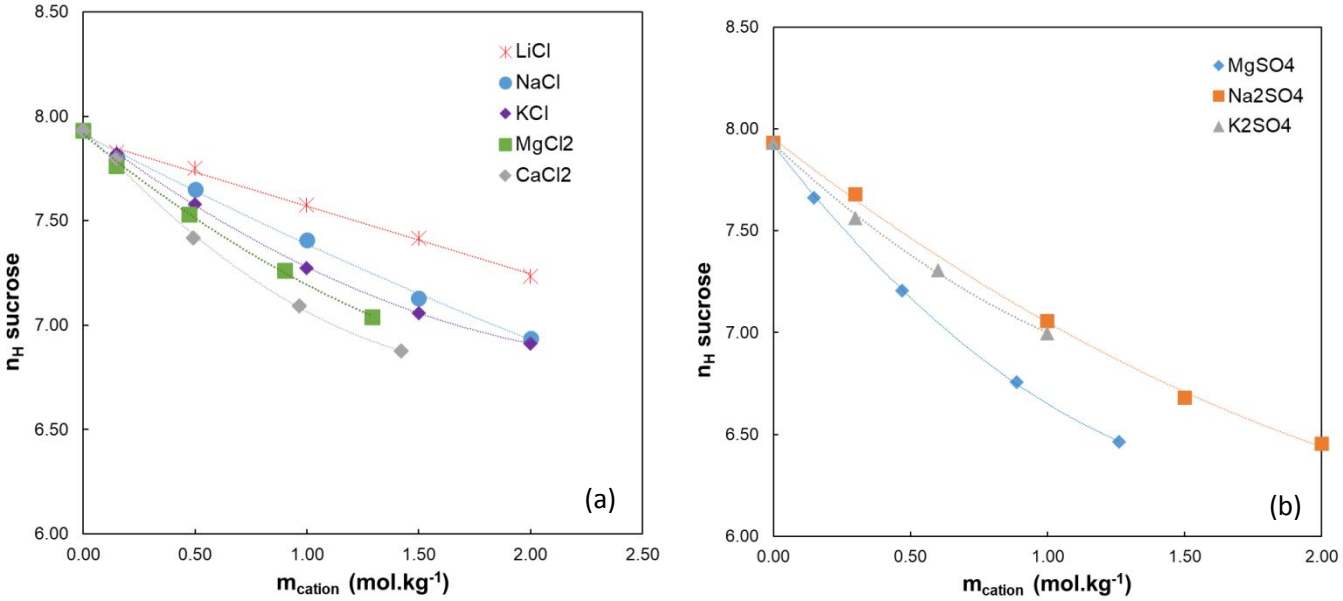


Figure S_2: Sucrose hydration number (n_H) versus the cation molality (m_E) for electrolytes containing Cl^- and SO_4^{2-}.

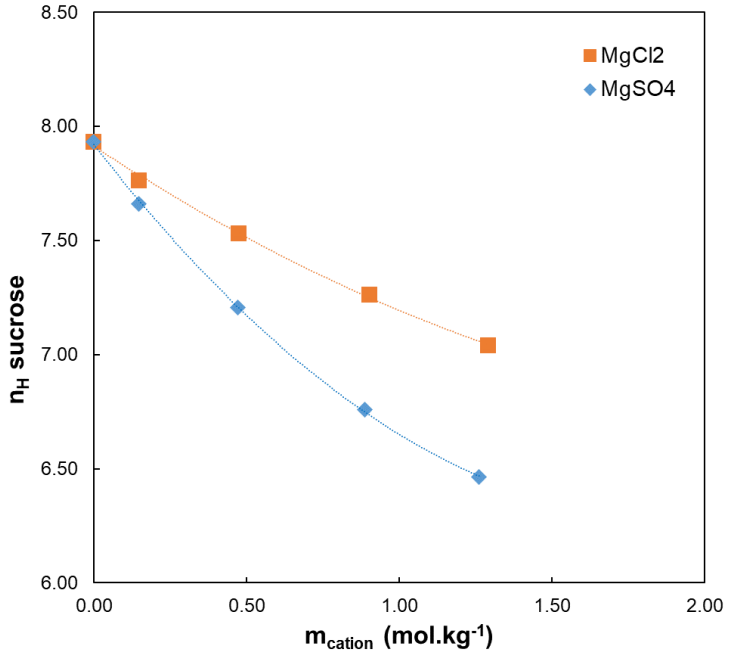
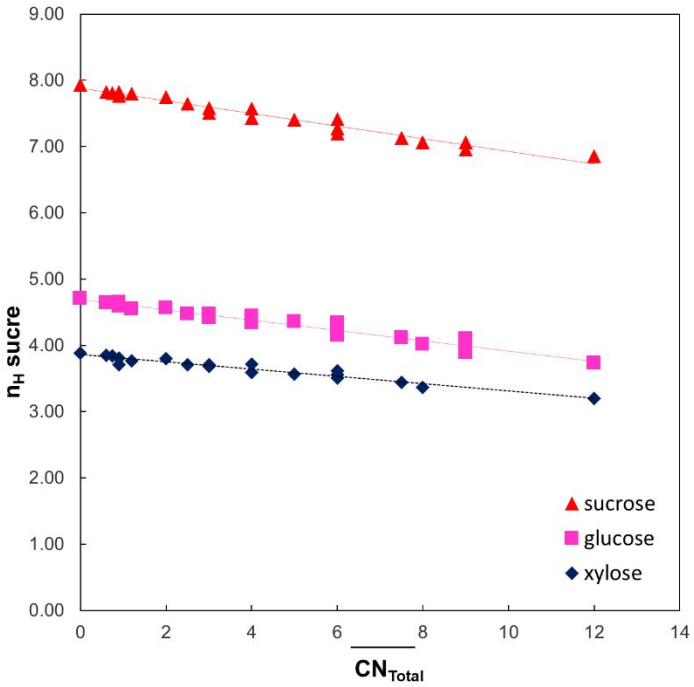


Figure S_3: Saccharide hydration number (n_H) versus $\overline{CN_{total}}$ for electrolytes containing Cl^-.

$\overline{CN_{total}} = CN_{cation}\, m_{cation}$; CN cation : cation coordination number et m_{cation} : cation molality.



Tables

Table S_1: Infinite-dilution apparent molar volumes $V^0_{\phi,S}$ ($cm^3.mol^{-1}$) of the saccharides in electrolyte solutions, electrolyte molality m_E ($mol.kg^{-1}$), slopes (S_S^*) ($cm^3.kg.mol^{-2}$) and saccharide hydration numbers at infinite dilution (n_H) at 298.15K.

	m_E		Xylose	Glucose	Sucrose
Water		n_H	3.88	4.72	7.93
LiCl	**0.1500**	$V_{\Phi S}^0$	95.65	112.21	211.86
		S_S^*	0.36	0.49	1.06
		n_H	3.85	4.64	7.83
	0.5000	$V_{\Phi S}^0$	95.79	112.44	212.11
		S_S^*	0.37	0.50	1.10
		n_H	3.80	4.57	7.75
	1.0000	$V_{\Phi S}^0$	96.07	112.85	212.69
		S_S^*	0.33	0.41	1.01
		n_H	3.72	4.44	7.57
	2.0000	$V_{\Phi S}^0$	96.78	113.49	213.82
		S_S^*	0.17	0.41	0.71
		n_H	3.50	4.25	7.23
NaCl	**0.1500**	$V_{\Phi S}^0$	95.68	112.20	211.93
		S_S^*	0.30	0.52	1.07
		n_H	3.84	4.64	7.81
	0.5000	$V_{\Phi S}^0$	96.11	112.73	212.44
		S_S^*	0.32	0.44	1.06
		n_H	3.71	4.48	7.65
	1.0000	$V_{\Phi S}^0$	96.57	113.13	213.25
		S_S^*	0.26	0.54	0.94
		n_H	3.57	4.36	7.41
	1.5000	$V_{\Phi S}^0$	97.00	113.92	214.16
		S_S^*	0.27	0.36	0.77
		n_H	3.44	4.12	7.13
	2.0000	$V_{\Phi S}^0$	97.37	114.32	214.80
		S_S^*	0.23	0.33	0.69
		n_H	3.32	4.00	6.94
KCl	**0.1500**	$V_{\Phi S}^0$	95.66	112.15	211.88
		S_S^*	0.39	0.57	1.05
		n_H	3.84	4.65	7.82
	0.5000	$V_{\Phi S}^0$	96.08	112.71	212.67
		S_S^*	0.34	0.48	0.91
		n_H	3.71	4.48	7.58
	1.0000	$V_{\Phi S}^0$	96.58	113.44	213.68
		S_S^*	0.26	0.34	0.67
		n_H	3.56	4.26	7.27
	2.0000	$V_{\Phi S}^0$		114.38	214.88

		S_S*		0.28	0.53
		n_H		3.98	6.91

	m_E		Xylose	Glucose	Sucrose
$MgCl_2$	**0.1500**	$V_{\Phi S}^0$	95.76	112.37	212.07
		S_S*	0.36	0.50	1.03
		n_H	3.81	4.59	7.76
	0.4744	$V_{\Phi S}^0$	96.17	112.92	212.84
		S_S*	0.34	0.49	0.97
		n_H	3.69	4.42	7.53
	0.9024	$V_{\Phi S}^0$	96.66	113.56	213.73
		S_S*	0.34	0.41	0.79
		n_H	3.54	4.23	7.26
	1.2907	$V_{\Phi S}^0$	97.04	114.35	214.46
		S_S*	0.30	0.21	0.72
		n_H	3.42	3.99	7.04
$CaCl_2$	**0.1492**	$V_{\Phi S}^0$	95.91	112.48	211.95
		S_S*	0.32	0.47	1.11
		n_H	3.77	4.55	7.80
	0.4911	$V_{\Phi S}^0$	96.38	113.20	213.21
		S_S*	0.33	0.44	0.88
		n_H	3.62	4.34	7.42
	0.9652	$V_{\Phi S}^0$	97.23	114.12	214.28
		S_S*	0.31	0.39	0.76
		n_H	3.37	4.06	7.09
	1.4231	$V_{\Phi S}^0$	97.68	115.10	215.00
		S_S*	0.29	0.19	0.77
		n_H	3.23	3.76	6.87

	m_E		Xylose	Glucose	Sucrose
Na_2SO_4	**0.1500**	$V_{\Phi S}^0$	96.15	112.82	212.34
		S_S*	0.30	0.45	1.12
		n_H	3.69	4.45	7.68
	0.5000	$V_{\Phi S}^0$	96.97	114.05	214.40
		S_S*	0.42	0.38	0.76
		n_H	3.45	4.08	7.06
	0.7500	$V_{\Phi S}^0$	97.64	114.90	215.64
		S_S*	0.34	0.26	0.53
		n_H	3.24	3.82	6.68
	1.0000	$V_{\Phi S}^0$	98.18	115.49	216.39
		S_S*	0.25	0.19	0.53
		n_H	3.08	3.64	6.45
K_2SO_4	**0.1500**	$V_{\Phi S}^0$		112.68	212.73
		S_S*		0.49	0.93
		n_H		4.49	7.56
	0.3000	$V_{\Phi S}^0$		113.41	213.58
		S_S*		0.42	0.83
		n_H		4.27	7.31
	0.5000	$V_{\Phi S}^0$	97.35	114.23	214.60
		S_S*	0.23	0.27	0.67
		n_H	3.33	4.02	7.00
$MgSO_4$	**0.1472**	$V_{\Phi S}^0$	95.86	112.45	212.40
		S_S*	0.42	0.54	1.00
		n_H	3.78	4.56	7.66
	0.4703	$V_{\Phi S}^0$	96.73	113.57	213.90
		S_S*	0.29	0.41	0.72
		n_H	3.52	4.22	7.21
	0.8880	$V_{\Phi S}^0$	97.61	114.63	215.38
		S_S*	0.23	0.25	0.54
		n_H	3.25	3.90	6.76
	1.2614	$V_{\Phi S}^0$		115.43	216.36
		S_S*		0.23	0.43
		n_H		3.66	6.46

Gaussian 09 full reference.

Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

Computational details

All DFT calculations were performed with Gaussian 09. Geometries were fully optimized in gas phase at 298.15 K and 1 atm, without symmetry constraints at the DFT level employing the hybrid density functional B3PW91[13]. For the Li, Na, K, Mg, Ca, H, O, Cl et S atoms, a double-zeta 6-31G[33] basis set augmented by a polarization function[34] were used.

Electronic energies, enthalpies and cartesian coordinates of the stationary points on the potential energy surfaces.

$Li^+ (H_2O)_n$

$Li^+ (H_2O)$

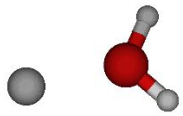


Figure S_4 : Li^+ optimized structure with 1 water molecule.

E = -83.706570
H = -83.705626

Li	-0.111316	0.000000	-0.109711
O	0.093477	0.000000	1.728684
H	0.925639	0.000000	2.219358
H	-0.609240	0.000000	2.391623

$Li^+ (H_2O)_2$

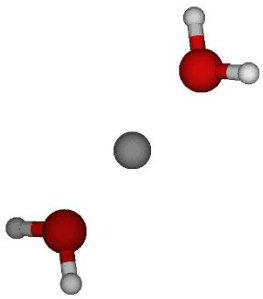


Figure S_5 : Li^+ optimized structure with 2 water molecules.

E = -152.844745
H = -152.843800

O	0.264866	-0.000038	2.035815

Li	-0.974695	0.000096	0.568741
H	1.227958	0.000043	1.972358
H	0.062564	-0.000087	2.979450
O	-2.219997	0.000230	-0.888932
H	-2.016761	-0.000009	-1.832399
H	-3.183108	-0.000234	-0.825908

$Li^+ (H_2O)_3$

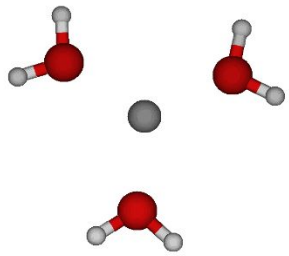


Figure S_6 : Li^+ optimized structure with 3 water molecules.

E = -229.251831
H = -229.250887

O	-0.015661	0.000316	1.767236
Li	-0.797324	0.000013	-0.022581
O	-2.737018	-0.000043	-0.251573
H	0.921694	0.003662	1.991296
H	-0.484930	-0.003957	2.609044
H	-3.222397	0.000064	-1.084201
H	-3.407319	0.000842	0.440933
O	0.369696	-0.000051	-1.588111
H	1.333484	-0.000302	-1.595281
H	0.102808	-0.000086	-2.514286

$Li^+ (H_2O)_4$

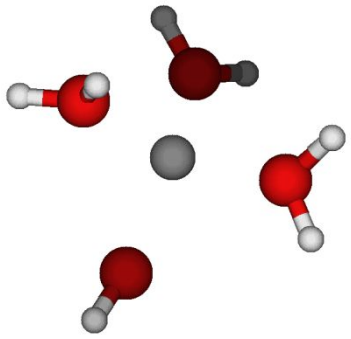


Figure S_7 : Li^+ optimized structure with 4 water molecules.

E = -305.646717
H = -305.645773

O	-0.136238	0.251761	1.702928
Li	-0.999037	-0.423053	0.037620
O	0.214014	-0.077729	-1.507242
O	-2.729947	0.505090	-0.303377
H	-0.057550	1.161152	2.009550
H	0.118122	-0.304697	2.446731
H	-2.944744	0.974517	-1.116444
H	-3.417021	0.738008	0.329778
H	1.043779	0.408212	-1.452921
H	0.203796	-0.493199	-2.375882
O	-1.332949	-2.376930	0.256510
H	-0.699965	-3.098257	0.177410
H	-2.204750	-2.786135	0.268660

$Li^+ (H_2O)_5$

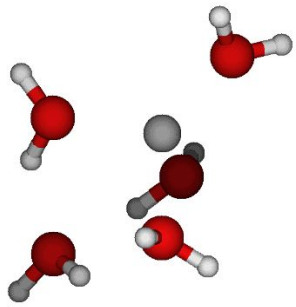


Figure S_8 : Li^+ optimized structure with 5 water molecules.

E = -382.034409
H = -382.033465

O	0.818674	-0.353806	2.164514
Li	-0.579747	-0.331782	0.769583
O	-2.770497	-0.297458	-1.415445
O	-1.535313	-2.005701	0.340495
O	-0.239573	0.638633	-0.918007
H	1.576102	0.237735	2.228437
H	0.956786	-1.039675	2.826480
H	-3.453102	-0.286575	-2.096229
H	-3.098431	0.221642	-0.663555
H	0.522887	0.651599	-1.504413
H	-1.021674	0.430446	-1.462768

H	-1.216760	-2.899761	0.183774
H	-2.097410	-1.760251	-0.418302
O	-2.329587	0.743057	1.203984
H	-2.222827	1.693479	1.337045
H	-2.851702	0.429746	1.953232

$Li^+ (H_2O)_6$

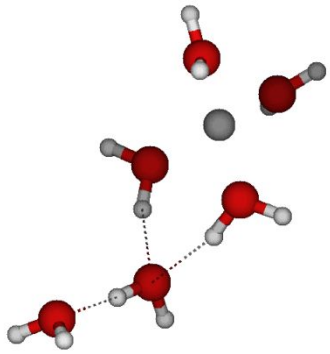


Figure S_9 : Li^+ optimized structure with 6 water molecules.

E = -458.426216
H = -458.425272

O	0.818674	-0.353806	2.164514
Li	-0.579747	-0.331782	0.769583
O	-1.535313	-2.005701	0.340495
O	-0.239573	0.638633	-0.918007
O	-2.329587	0.743057	1.203984
O	-2.770497	-0.297458	-1.415445
H	1.576102	0.237735	2.228437

H	0.956786	-1.039675	2.826480
H	-3.453102	-0.286575	-2.096229
H	-3.098431	0.221642	-0.663555
H	0.522887	0.651599	-1.504413
H	-1.021674	0.430446	-1.462768
H	-1.216760	-2.899761	0.183774
H	-2.097410	-1.760251	-0.418302
H	-2.222827	1.693479	1.337045
H	-2.851702	0.429746	1.953232
O	-0.328571	-1.170157	-0.716679
H	0.219259	-0.791961	-1.394432
H	-1.033652	-1.664124	-1.118371

$Li^+ (H_2O)_7$

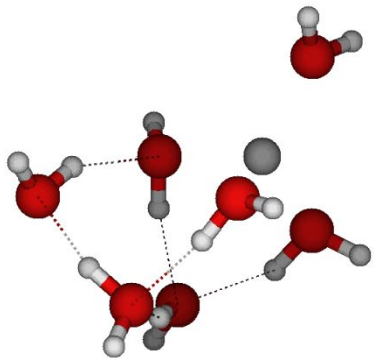


Figure S_{10} : Li^+ optimized structure with 7 water molecules.

E = -534.817476
H = -534.816532

O	1.267867	-1.730082	2.266237
Li	0.105597	-1.119374	0.781848
O	-0.727542	0.777359	-1.815988

O	1.035367	-1.135429	-0.972838
O	-1.697216	-1.908177	0.716444
O	-3.060269	-0.166446	-0.885643
O	-2.983125	1.569231	1.042557
H	2.217084	-1.881884	2.211940
H	0.992714	-2.032065	3.137948
H	-3.894755	-0.287194	-1.352311
H	-3.207707	0.514214	-0.162876
H	-0.743801	1.459815	-2.495749
H	-1.652272	0.446208	-1.694956
H	-1.899103	-2.846332	0.653436
H	-2.315901	-1.439258	0.114612
H	-3.466597	1.455071	1.867534
H	-2.036419	1.456038	1.250643
H	1.321227	-1.884808	-1.503688
H	0.548122	-0.530396	-1.565564
O	-0.262386	0.929407	0.815696
H	-0.326617	1.120988	-0.152082
H	0.435036	1.494700	1.168060

$Li^{+}\ (H_2O)_8$

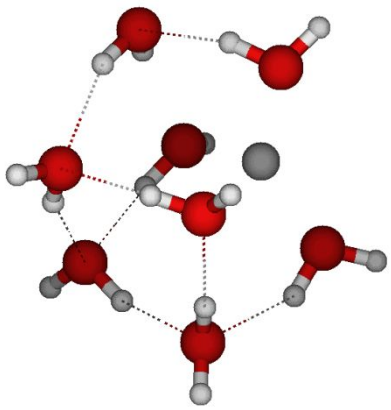


Figure S_{11} : Li^+ optimized structure with 8 water molecules.

E = -611.204611
H = -611.203667

O	1.500144	-1.216588	1.567900
Li	-0.428585	-0.979776	1.606160
O	-1.365364	-2.094219	0.169051
O	1.203842	-1.648857	-1.020402
O	-0.331697	1.005299	0.911500
O	-0.376644	0.698804	-1.723824
O	-2.890308	-0.153512	-0.984986
O	-2.943566	1.174151	1.387008
H	1.626137	-1.390287	0.596943
H	2.127166	-1.766497	2.046266
H	-3.703922	-0.279124	-1.486461
H	-3.112418	0.378793	-0.183328
H	-0.244658	1.361206	-2.411353
H	-1.322599	0.440140	-1.739082
H	-1.814468	-2.890255	0.475493
H	-2.034933	-1.556581	-0.310639

H	-3.444380	1.972049	1.592094
H	-1.994588	1.425363	1.307635
H	0.388824	-2.160357	-0.898874
H	0.900721	-0.847125	-1.476662
H	-0.208723	1.036551	-0.072044
H	0.478567	1.347343	1.309410
O	-1.817035	-0.806213	2.992647
H	-1.827033	-0.855346	3.952799
H	-2.467139	-0.133826	2.719425

$Li^+ (H_2O)_9$

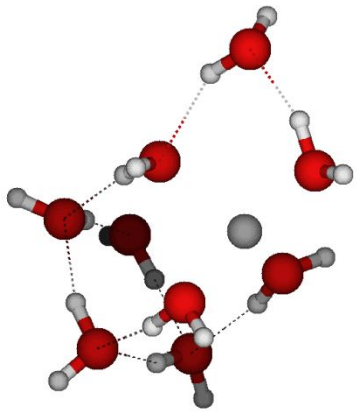


Figure S_{12} : Li^+ optimized structure with 9 water molecules.

E = -687.593539
H = -687.592595

O	0.675643	-3.177079	1.664390
Li	-0.567893	-1.693651	1.464221
O	-1.648918	-0.869320	2.935401
O	-1.713868	-1.985469	-0.094443
O	-0.622210	2.116917	0.442156

O	2.879162	-1.833719	1.106277
O	-1.416401	1.477811	-1.934439
O	-2.879376	1.247528	1.592296
O	-3.452683	0.047319	-0.781116
H	1.594448	-2.856308	1.476838
H	0.742179	-3.899364	2.294255
H	-4.370067	-0.100514	-1.035711
H	-3.455061	0.494321	0.097331
H	-1.605858	2.090416	-2.652054
H	-2.238277	0.977605	-1.751387
H	-1.527979	-2.656738	-0.756770
H	-2.391939	-1.382350	-0.456904
H	-3.428748	1.903219	2.036893
H	-2.067652	1.717370	1.268681
H	3.344410	-1.969438	0.274406
H	2.362511	-1.014915	1.006961
H	-0.856448	1.967902	-0.526668
H	-0.228905	2.994155	0.511697
H	-2.201417	-1.385655	3.530676
H	-2.201922	-0.133239	2.604148
O	0.730664	-0.063196	1.406722
H	0.812529	0.145414	2.345997
H	0.368485	0.753296	0.992665

$Li^{+}(H_2O)_{10}$

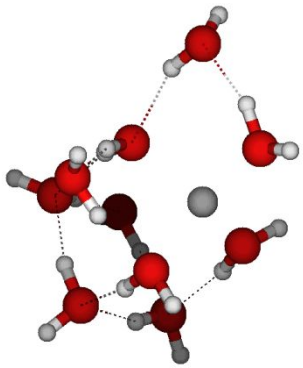


Figure S_{13} : Li^+ optimized structure with 10 water molecules.

E = -763.981303
H = -763.980359

O	0.543817	-3.212290	1.621355
Li	-0.677924	-1.727979	1.379449
O	-2.004733	-1.051750	2.815261
O	0.583020	-0.134389	1.441446
O	-1.813697	-2.039255	-0.195171
O	2.750367	-1.819962	1.359076
O	-3.435565	0.054489	-0.991793
O	-2.960293	1.141191	1.459551
O	-0.723529	2.098343	0.413468
O	-1.375267	1.552219	-2.038891
H	1.476247	-2.877986	1.541269
H	0.565202	-4.066769	2.058232
H	-4.339847	-0.092242	-1.290429
H	-3.480843	0.479661	-0.104326
H	-1.545196	2.185550	-2.743218
H	-2.195908	1.036735	-1.905540
H	-1.499387	-2.622405	-0.892420

H	-2.419533	-1.390736	-0.606175
H	-3.511083	1.791652	1.910554
H	-2.128758	1.613432	1.173512
H	3.289752	-1.896595	0.565433
H	2.191134	-1.025668	1.242941
H	-0.895308	2.005591	-0.571455
H	-0.346800	2.971739	0.567289
H	-2.703207	-1.647997	3.107385
H	-2.448945	-0.264626	2.422623
H	0.572958	0.094762	2.407292
H	0.297030	0.680457	0.982035
O	0.129302	0.274031	4.029607
H	-0.671528	-0.277254	3.994111
H	0.704946	-0.115078	4.696697

$Li^+ (H_2O)_{11}$

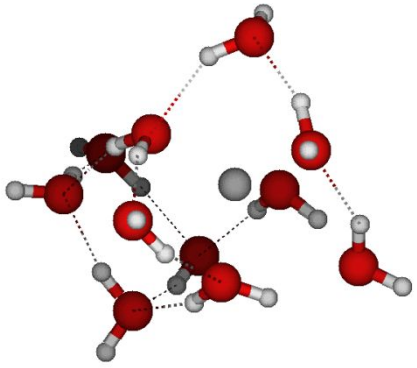


Figure S_{14} : Li^+ optimized structure with 11 water molecules.

E = -840.366244
H = -840.365300

O	0.543817	-3.212290	1.621355

Li	-0.677924	-1.727979	1.379449
O	-1.813697	-2.039255	-0.195171
O	0.583020	-0.134389	1.441446
O	-2.004733	-1.051750	2.815261
O	2.750367	-1.819962	1.359076
O	0.129302	0.274031	4.029607
O	-2.960293	1.141191	1.459551
O	-0.723529	2.098343	0.413468
O	-1.375267	1.552220	-2.038891
O	-3.435565	0.054489	-0.991793
H	1.476247	-2.877986	1.541269
H	0.565202	-4.066769	2.058232
H	-4.339847	-0.092242	-1.290429
H	-3.480843	0.479661	-0.104326
H	-1.545196	2.185551	-2.743218
H	-2.195908	1.036736	-1.905540
H	-1.499387	-2.622405	-0.892420
H	-2.419533	-1.390736	-0.606175
H	-3.511083	1.791652	1.910554
H	-2.128758	1.613432	1.173512
H	3.289752	-1.896595	0.565433
H	2.191134	-1.025668	1.242941
H	-0.895308	2.005591	-0.571455
H	-0.346800	2.971739	0.567290
H	-2.703207	-1.647997	3.107385
H	-2.448945	-0.264626	2.422623
H	0.572958	0.094762	2.407292
H	0.297030	0.680457	0.982035

H	-0.671528	-0.277254	3.994111
H	0.704946	-0.115078	4.696697
O	-1.747677	-3.079940	1.326852
H	-2.631160	-3.295125	1.601901
H	-1.124693	-3.472344	1.927194

$Na^+ (H_2O)$

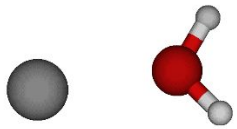


Figure S_{15} : Na^+ optimized structure with 1 water molecule.

E = -76.408209
H = -76.407265

Na	-0.107909	0.000000	-0.183683
O	0.098617	0.000000	2.030680
H	0.914407	0.000000	2.546154
H	-0.606556	0.000000	2.689404

$Na^+ (H_2O)_2$

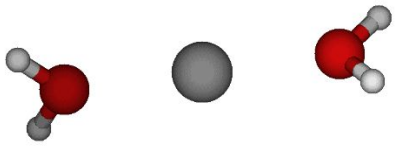


Figure S_{16} : Na^+ optimized structure with 2 water molecules.

E = -152.813067
H = -152.812123

O	0.029916	-0.257099	2.441534
Na	0.427524	0.807546	0.510660
H	0.620120	-0.842347	2.930850
H	-0.777446	-0.226394	2.968434
O	0.830130	1.883065	-1.415490
H	0.708693	1.551577	-2.312960

H	1.165296	2.780350	-1.527864

$Na^+ (H_2O)_3$

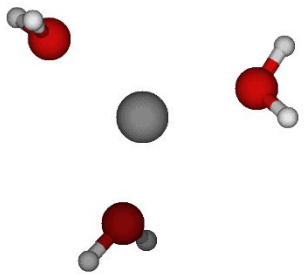


Figure S_{17} : Na^+ optimized structure with 3 water molecules.

E = -229.212399
H = -229.211455

O	-0.165035	-0.754009	1.920779
Na	0.577092	1.216110	1.076036
O	0.593473	1.552682	-1.166871
H	0.308273	-1.358884	2.503103
H	-1.022868	-1.168666	1.775210
H	1.028687	1.014541	-1.837691
H	0.167822	2.265209	-1.656898
O	1.303266	2.846840	2.475611
H	0.818172	3.256988	3.200511
H	2.164236	3.280124	2.475511

$Na^+ (H_2O)_4$

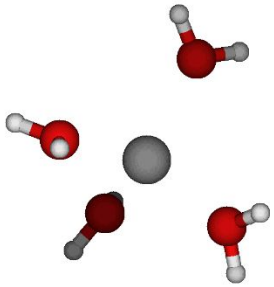


Figure S_{18} : Na^+ optimized structure with 4 water molecules.

E = -305.604745
H = -305.603801

O	-0.382750	-0.545501	1.692928
Na	0.934957	1.048677	0.673539
O	-0.124864	1.887823	-1.193874
O	1.334490	2.782080	2.141326
H	-0.119166	-1.206129	2.342386
H	-1.313722	-0.721761	1.519531
H	0.109006	1.715182	-2.112205
H	-0.857234	2.512057	-1.234491
H	1.158025	2.786275	3.088240
H	1.662323	3.665789	1.943151
O	2.931565	0.066716	0.065436
H	3.815668	0.412433	0.228777
H	3.070467	-0.787504	-0.357308

$Na^+ (H_2O)_5$

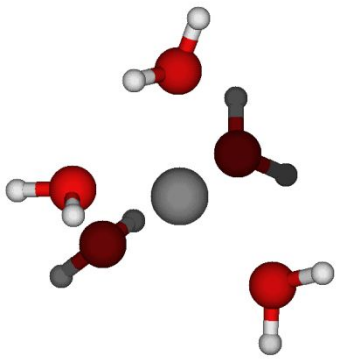


Figure S_{19} : Na^+ optimized structure with 5 water molecules.

E = -381.989449
H = -381.988505

O	-0.351339	-0.663960	1.733218
Na	1.151766	0.907002	0.938066
O	0.561394	1.955909	-1.012212
O	0.873537	2.871389	2.448242
O	2.263717	-0.203846	-1.005877
H	-0.162566	-1.422804	2.295375
H	-1.299728	-0.698530	1.569273
H	1.089679	1.402406	-1.604373
H	0.053592	2.559131	-1.561711
H	0.305805	2.905974	3.226576
H	0.836033	3.757232	2.069393
H	3.219546	-0.128191	-1.107234
H	2.040154	-1.070837	-1.363185
O	3.049468	1.204140	2.189869
H	3.905394	0.956748	2.550341
H	2.749043	1.986015	2.673887

$Na^+ (H_2O)_6$

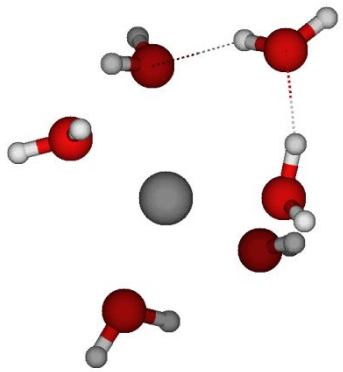


Figure S_{20} : Na^+ optimized structure with 6 water molecules.

E = -458.376198
H = -458.375254

O	0.040906	-0.630113	1.083937
Na	1.190545	1.375132	0.660449
O	0.898207	2.252238	-1.402381
O	2.780869	1.329131	2.469564
O	0.642517	3.049338	2.406349
O	1.793090	-0.310461	-0.970703
H	0.452902	-0.934059	1.934270
H	-0.884432	-0.893263	1.112740
H	1.161815	1.442283	-1.864777
H	0.501454	2.838280	-2.052377
H	-0.088937	2.932059	3.025007
H	0.662309	3.995787	2.219237
H	2.465385	-0.901434	-1.322985
H	1.144376	-0.862203	-0.497320
H	3.730776	1.476477	2.537973
H	2.342807	2.097170	2.873955
O	1.360552	-0.947698	3.345966

H	2.052899	-0.272087	3.235486
H	1.789612	-1.742576	3.678421

$Na^+ (H_2O)_7$

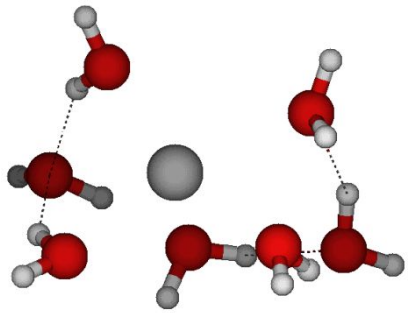


Figure S_{21} : Na^+ optimized structure with 7 water molecules.

E = -534.765590
H = -534.764646

O	0.228849	-0.349015	0.911301
Na	1.930438	1.373728	0.855610
O	0.606690	1.608760	-1.094897
O	2.781638	0.922782	3.204514
O	1.439062	-1.020550	-1.424965
O	0.852185	2.654214	2.627368
O	0.197976	0.136408	3.591189
H	0.027802	-0.466488	1.861107
H	-0.505968	0.150723	0.534183
H	0.821462	0.778885	-1.560887
H	0.437723	2.268180	-1.774660
H	0.291603	1.992844	3.075749
H	0.401021	3.501416	2.702304
H	1.272484	-1.774364	-2.000601

H	0.976574	-1.185853	-0.579831
H	3.650523	0.708886	3.562098
H	2.564968	1.828657	3.475035
H	1.170504	0.122214	3.701306
H	-0.191363	-0.257929	4.379474
O	3.575074	0.261572	-0.272988
H	4.476867	0.303769	-0.601373
H	3.088031	-0.356537	-0.849395

$Na^+ (H_2O)_8$

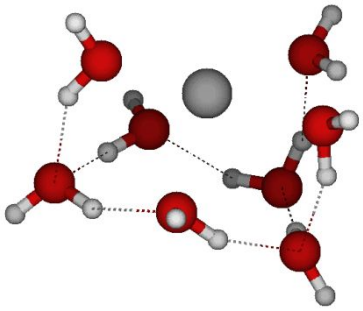


Figure S_{22} : Na^+ optimized structure with 8 water molecules.

E = -611.160863
H = -611.159919

O	-0.002982	0.005891	0.950253
Na	1.660429	1.844663	0.610506
O	3.283857	0.052606	0.348702
O	1.082824	1.684698	-1.591248
O	0.476361	2.733103	2.645725
O	3.118226	0.260307	3.121544
O	1.322293	-1.055994	-1.117717

O	0.575109	0.196453	3.540068
H	0.082636	-0.152988	1.922385
H	-0.926913	0.233010	0.797737
H	1.110950	0.735191	-1.805918
H	1.032124	2.160468	-2.424796
H	0.345384	1.912792	3.175745
H	-0.234987	3.339693	2.875112
H	1.172497	-1.920381	-1.515090
H	0.695409	-0.949691	-0.367496
H	3.306765	-0.091106	2.230610
H	3.361438	1.201304	3.048147
H	1.583718	0.138403	3.484881
H	0.292847	-0.270750	4.333850
H	4.163748	0.117041	-0.037917
H	2.768815	-0.553131	-0.230541
O	3.080720	2.943616	2.247464
H	3.725311	3.647299	2.375854
H	2.252238	3.209537	2.694728

$Na^+ (H_2O)_9$

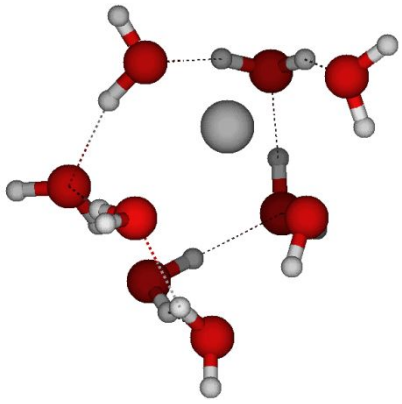


Figure S_{23} : Na^+ optimized structure with 9 water molecules.

E = -687.547731
H = -687.546786

O	-0.620989	-0.405963	0.961132
Na	2.676819	2.224305	0.554858
O	1.067297	1.981661	-1.224820
O	3.581491	2.936636	2.647916
O	3.517707	0.070497	0.283747
O	0.994587	2.736662	2.057098
O	0.593940	0.376104	3.288746
O	3.179969	0.097074	3.097255
O	1.188553	-0.626251	-0.780539
H	-0.261653	-0.317354	1.869660
H	-1.038033	0.460463	0.784886
H	1.057974	0.987974	-1.276279
H	1.086070	2.306709	-2.131819
H	0.756614	1.959750	2.616516
H	0.155074	2.959601	1.617181
H	1.018735	-1.363180	-1.378068
H	0.452373	-0.636749	-0.055000

H	3.409664	-0.177703	2.191423
H	3.529193	1.001626	3.171059
H	1.569620	0.146633	3.318021
H	0.236378	0.254663	4.175043
H	4.324955	-0.305124	-0.083635
H	2.753511	-0.398123	-0.140529
H	4.208597	3.492503	3.123001
H	2.686409	3.253540	2.867168
O	-1.172291	2.273938	0.413482
H	-2.016724	2.653937	0.147342
H	-0.571461	2.302931	-0.357336

$Na^+ (H_2O)_{10}$

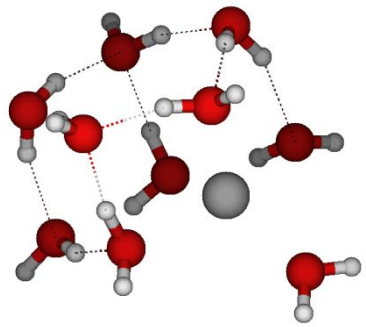


Figure S_{24} : Na^+ optimized structure with 10 water molecules.

E = -763.939139
H = -763.938195

O	-0.713395	-0.451660	1.174553
O	0.945889	-0.810328	-0.693857
O	0.807884	1.736495	-1.384391
Na	2.580114	2.284537	0.259286
O	0.941808	2.609423	1.981035

O	3.307689	0.028280	0.213019
O	3.497321	3.007984	2.461216
O	0.718542	0.308351	3.379573
O	3.290298	0.214402	3.029511
O	-1.243700	2.209618	0.384311
H	-0.262151	-0.334380	2.039241
H	-1.123812	0.413062	0.981389
H	0.812742	0.743117	-1.325080
H	0.756681	1.955623	-2.321046
H	0.763415	1.858680	2.595084
H	0.073934	2.809438	1.584179
H	0.744935	-1.605795	-1.199130
H	0.264652	-0.752700	0.079387
H	3.419927	-0.060229	2.102761
H	3.546801	1.154905	3.031128
H	1.711563	0.151635	3.332917
H	0.442685	0.169310	4.291770
H	4.088937	-0.361357	-0.193705
H	2.525668	-0.476590	-0.125555
H	4.023883	3.629344	2.974578
H	2.555888	3.228563	2.608838
H	-2.077173	2.608380	0.112635
H	-0.667145	2.148476	-0.407343
O	3.823810	3.808901	-0.956882
H	3.728665	4.166166	-1.845586
H	4.593389	4.254095	-0.586680

$Na^+ (H_2O)_{11}$

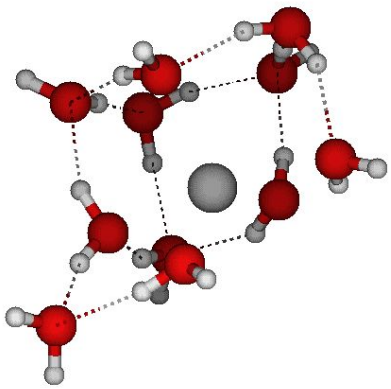


Figure S_{25} : Na^+ optimized structure with 11 water molecules.

E = -840.327442
H = -840.326498

O	-0.741788	-0.163158	0.637903
O	1.318745	-0.558187	-0.791125
O	1.695511	2.093765	-0.854969
Na	2.959853	1.955694	1.235880
O	3.439116	3.704385	-2.446038
O	3.356955	-0.364635	0.909016
O	0.960304	2.350940	2.530043
O	3.331067	2.153353	3.646338
O	0.039976	-0.084977	3.268548
O	2.565959	-0.605128	3.601147

O	-0.662042	2.639153	0.343269
H	-0.553647	-0.283442	1.593902
H	-0.944723	0.787221	0.537451
H	1.581739	1.146361	-1.104167
H	2.161479	2.552735	-1.574286
H	0.508490	1.556799	2.897991
H	0.292853	2.766737	1.953548
H	1.155305	-1.234685	-1.456967
H	0.465940	-0.478906	-0.223770
H	2.912675	-0.754178	2.701437
H	2.946700	0.254528	3.857466
H	0.973449	-0.408849	3.456997
H	-0.512780	-0.336360	4.015837
H	4.165990	-0.816262	0.647247
H	2.656148	-0.629246	0.258789
H	3.823742	2.613491	4.333304
H	2.431524	2.536253	3.617777
H	-1.323001	3.209697	-0.061905
H	0.115270	2.595851	-0.259799
H	3.112621	4.565678	-2.733219
H	3.956156	3.363923	-3.185942
O	4.427649	3.382313	0.202313
H	5.225963	3.851143	0.460902
H	4.245199	3.625365	-0.721121

$Na^+ (H_2O)_{12}$

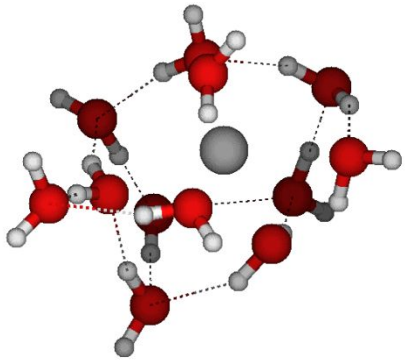


Figure S_{26} : Na^+ optimized structure with 12 water molecules.

E = -916.709122
H = -916.708178

O	-0.964290	0.054262	0.723736
O	0.944283	-0.667761	-0.792290
O	3.006080	-0.773544	0.898599
Na	3.201359	1.620595	1.117559
O	4.135875	3.880922	0.162605
O	1.241410	2.299199	2.488114
O	3.552919	1.780554	3.576299
O	1.796660	1.861625	-0.889989
O	-0.403875	2.792611	0.363713
O	-0.025612	0.056139	3.308428
O	2.388630	-0.840839	3.612880
O	3.413526	3.510436	-2.551338
H	-0.734036	-0.084996	1.667843
H	-1.001944	1.024451	0.616435
H	1.521116	0.942086	-1.120304
H	2.224689	2.271901	-1.659058
H	0.686227	1.579906	2.870261

H	0.629521	2.805639	1.923575
H	0.658255	-1.323925	-1.436412
H	0.137562	-0.451962	-0.196271
H	2.653869	-1.055991	2.697432
H	2.895859	-0.032941	3.814974
H	0.853402	-0.403697	3.489252
H	-0.582660	-0.067541	4.083973
H	3.768929	-1.247648	0.551853
H	2.263282	-0.931601	0.264105
H	4.062285	2.170180	4.293632
H	2.706008	2.269047	3.509387
H	-0.969668	3.445074	-0.060969
H	0.345031	2.591599	-0.245786
H	3.056152	4.163947	-3.164413
H	4.157231	3.101907	-3.011083
H	4.244464	4.776189	0.498612
H	3.875590	3.960778	-0.773416
O	5.437045	1.533578	0.320516
H	6.278408	1.292966	0.719320
H	5.420036	2.504727	0.265497

$Na^+ (H_2O)_{13}$

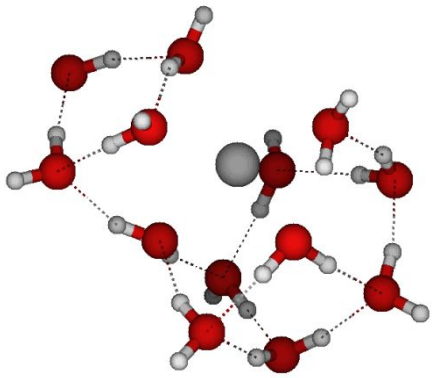


Figure S_{27} : Na^+ optimized structure with 13 water molecules.

E = -993.105967
H = -993.102023

O	-1.206768	0.164724	0.972778
O	0.596494	-0.738747	-0.578048
O	2.729125	-0.857389	0.994766
Na	2.979845	1.523915	1.157870
O	5.431839	1.406495	0.241138
O	1.561904	1.762554	-0.786388
O	1.157136	2.332993	2.607910
O	3.505957	1.731993	3.569939
O	4.016657	3.628757	0.181026
O	-0.512708	2.853040	0.518756
O	-0.201825	0.190170	3.539208
O	2.186927	-0.817931	3.739175
O	3.345069	3.070904	-2.367001
H	-0.964778	0.043843	1.915706
H	-1.196104	1.131790	0.832674
H	1.231173	0.865915	-1.017218
H	2.023967	2.156874	-1.554012

H	0.575001	1.664184	3.037724
H	0.557134	2.847005	2.035080
H	0.243390	-1.411709	-1.169414
H	-0.168965	-0.444787	0.037725
H	2.394979	-1.057048	2.815270
H	2.748882	-0.039376	3.905952
H	0.658129	-0.308699	3.692997
H	-0.734846	0.106240	4.336634
H	3.408454	-1.474850	0.705321
H	1.943529	-0.999101	0.403867
H	4.059898	2.108131	4.261157
H	2.675344	2.252743	3.537001
H	-1.048905	3.535450	0.102601
H	0.196924	2.589810	-0.116216
H	3.260276	3.667948	-3.117878
H	4.110973	2.453679	-2.559028
H	4.171823	4.537944	0.455702
H	3.756931	3.646745	-0.772253
H	6.247497	1.266239	0.734413
H	5.231380	2.369479	0.280345
O	5.402822	1.482823	-2.503972
H	5.558738	1.283569	-1.556181
H	5.421268	0.645743	-2.977753

$Na^+ (H_2O)_{14}$

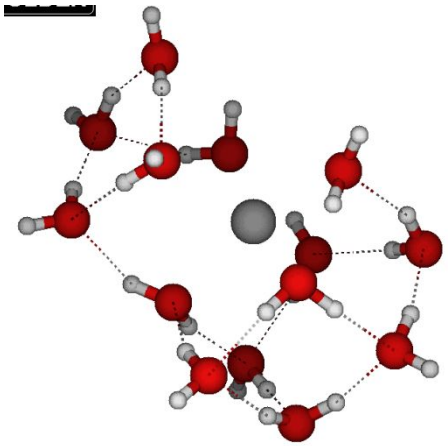


Figure S_{28} : Na^+ optimized structure with 14 water molecules.

E = -1069.489185
H = -1069.488240

O	-1.534817	0.372645	1.172990
O	0.053553	-0.646881	-0.558213
O	2.171026	-1.022638	1.091620
Na	2.711016	1.321388	1.085784
O	1.210747	1.745860	-0.777488
O	1.122208	2.335286	2.669688
O	3.461049	1.436083	3.456110
O	4.008103	3.297907	0.138127
O	6.376650	2.045238	-0.434633
O	-0.641927	3.016866	0.690860
O	3.127316	2.911240	-2.406121
O	5.143445	1.184899	-2.617942
O	-0.332665	0.289497	3.658122
O	1.912232	-0.995988	3.820366
H	-1.217123	0.209742	2.086663
H	-1.444065	1.336434	1.047907

H	0.790889	0.871217	-0.964110
H	1.681214	2.063194	-1.569257
H	0.525950	1.687431	3.115816
H	0.521035	2.898434	2.148143
H	-0.406886	-1.245664	-1.155259
H	-0.631177	-0.313784	0.120298
H	2.030638	-1.283401	2.892176
H	2.556578	-0.271548	3.909892
H	0.475491	-0.302502	3.787213
H	-0.836116	0.271368	4.478649
H	2.984461	-1.210433	0.599581
H	1.417855	-1.132841	0.470394
H	4.107653	1.736804	4.102123
H	2.695385	2.045475	3.497160
H	-1.174074	3.722429	0.309902
H	-0.019872	2.692668	-0.003624
H	3.035419	3.557513	-3.114277
H	3.840039	2.278343	-2.674842
H	3.942737	4.187369	0.502864
H	3.652355	3.343585	-0.781340
H	7.208568	2.503527	-0.277710
H	5.650506	2.622860	-0.108830
H	5.804751	1.550640	-1.978653
H	5.621186	0.835317	-3.377497
O	4.431749	-0.013760	-0.156836
H	5.313431	0.220578	0.165112
H	4.518506	0.105034	-1.118568

$Na^+ (H_2O)_{15}$

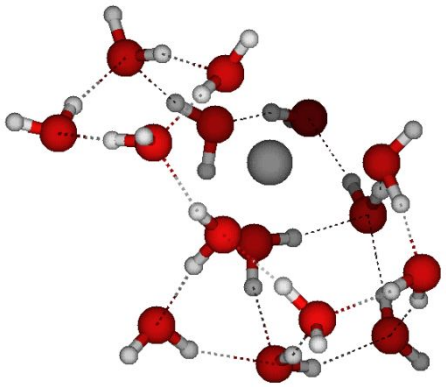


Figure S_{29} : Na^+ optimized structure with 15 water molecules.

E = -1145.872115
H = -1145.871171

O	-1.071925	0.218907	0.740908
O	0.049737	0.455214	-1.759747
O	1.402085	2.487493	-0.649398
Na	2.933408	1.635589	0.999909
O	4.315883	-1.618200	3.198950
O	0.003297	2.557943	3.506582
O	2.524459	2.144913	3.245276
O	4.240607	-0.406224	0.694426
O	4.700964	2.952297	-0.075257
O	-0.739454	2.977481	0.867432
O	-0.747317	-0.157246	3.519303
O	1.920689	-0.546931	3.696170
O	3.322990	3.715227	-2.215672

O	4.165664	1.625903	-3.508000
O	5.706754	0.767389	-1.393177
H	-1.205436	-0.117528	1.647228
H	-1.105792	1.194306	0.823557
H	0.957322	1.758502	-1.157768
H	1.870847	3.046136	-1.300099
H	-0.388921	1.670305	3.632402
H	-0.336837	2.864672	2.643307
H	-0.520238	0.524628	-2.531524
H	-0.507988	0.120228	-1.032996
H	2.746436	-1.093657	3.665964
H	2.235713	0.379337	3.746740
H	0.160218	-0.496816	3.696244
H	-1.318858	-0.532171	4.197953
H	4.479199	-1.285127	2.293444
H	4.508586	-2.560617	3.182344
H	3.023169	2.623551	3.915576
H	1.547903	2.385940	3.389907
H	-1.379520	3.616459	0.537819
H	0.046893	2.996488	0.264935
H	3.338913	4.547629	-2.699257
H	3.624205	2.989718	-2.839695
H	5.261371	3.601736	0.363208
H	4.264103	3.413156	-0.838294
H	6.662610	0.657145	-1.447496
H	5.539838	1.583230	-0.867096
H	4.786999	1.181574	-2.893037
H	4.545960	1.571374	-4.389660

H	4.796918	-0.347335	-0.101674
H	3.359473	-0.740848	0.436973
O	1.634986	-0.325514	1.000398
H	0.687799	-0.237382	0.772016
H	1.655986	-0.552662	1.957132

$Na^+ (H_2O)_{16}$

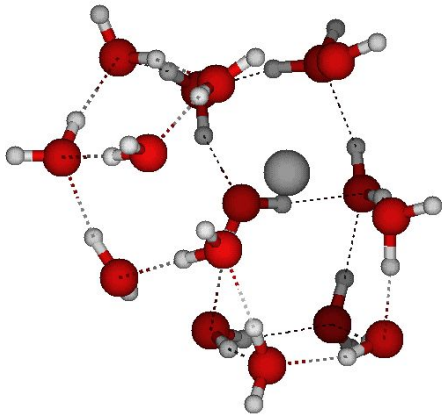


Figure S_{30} : Na^+ optimized structure with 16 water molecules.

E = -1222.265425
H = -1222.264481

O	-0.604666	0.162017	0.397265
O	0.606327	1.297568	-1.959020
O	1.373555	3.182438	-0.310569
Na	2.864457	2.256566	1.282495
O	1.971389	2.507872	3.466598
O	2.008574	0.114314	0.985641
O	4.200288	-1.388813	0.502191
O	4.723711	2.343724	-0.315455
O	-0.582013	2.326960	3.449047

O	3.451158	3.807031	-2.170231
O	3.087866	1.271421	-3.230620
O	-1.063113	2.896708	0.784237
O	2.159919	-0.212366	3.679246
O	4.832482	-0.449914	2.818612
O	-0.564845	-0.477611	3.198797
O	5.045425	0.158460	-1.741498
H	-0.842046	-0.281924	1.230677
H	-0.903123	1.089388	0.504592
H	1.091522	2.440924	-0.926987
H	1.840193	3.795581	-0.902898
H	-0.748118	1.363477	3.452002
H	-0.897553	2.644539	2.579683
H	1.406328	1.011259	-2.437079
H	0.225118	0.534694	-1.500890
H	3.096739	-0.486065	3.597172
H	2.182506	0.762169	3.814324
H	0.363963	-0.626085	3.471544
H	-1.105573	-1.050361	3.753582
H	4.684213	-0.862211	1.901544
H	5.492500	-0.997017	3.258944
H	2.251742	3.095321	4.176261
H	0.953162	2.507258	3.493104
H	-1.806758	3.357634	0.381747
H	-0.239126	3.252120	0.372739
H	3.681232	4.494302	-2.804362
H	3.292294	2.984872	-2.688485
H	5.284412	2.570860	0.447831

H	4.546844	3.109421	-0.900978
H	5.921787	0.028027	-2.120502
H	5.082968	0.980472	-1.182201
H	3.803231	0.740455	-2.799719
H	3.099279	1.051043	-4.168457
H	4.613804	-1.019914	-0.298996
H	3.292750	-1.011709	0.497457
H	1.073096	0.097982	0.662518
H	1.957750	-0.136432	1.936029
O	5.170383	2.178395	2.299550
H	5.596142	2.644843	3.025310
H	5.193459	1.216431	2.537912

$Na^+ (H_2O)_{17}$

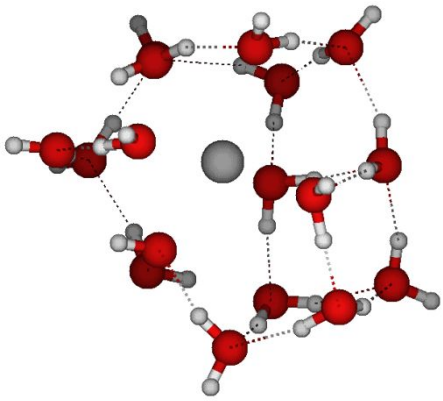


Figure S_{31} : Na^+ optimized structure with 17 water molecules.

E = -1298.650881
H = -1298.649937

O	-0.572190	0.039608	0.357235
O	2.033779	0.370482	0.994717
Na	2.726209	2.609274	1.308174

O	0.983137	3.142030	-0.330951
O	1.766652	2.527530	3.516844
O	5.079234	2.213886	-0.401771
O	5.135087	2.150038	2.271085
O	-0.767426	2.086638	3.476533
O	0.456000	1.217055	-2.001129
O	5.020097	0.047427	-1.800250
O	3.457794	3.932135	-2.109004
O	-1.361287	2.659618	0.846470
O	3.025325	1.342033	-3.044589
O	4.791706	-0.427591	2.914967
O	4.158581	-1.257978	0.570261
O	2.115126	-0.181470	3.657250
O	-0.531275	-0.699949	3.097463
H	-0.753705	-0.471020	1.167487
H	-1.002558	0.908604	0.502754
H	0.792911	2.402549	-0.989403
H	1.273388	3.886848	-0.870866
H	-0.855447	1.113759	3.445140
H	-1.121236	2.402253	2.621133
H	1.327998	0.986006	-2.373149
H	0.133120	0.462762	-1.482854
H	3.061659	-0.430273	3.595953
H	2.098836	0.787111	3.829216
H	0.406244	-0.751259	3.381517
H	-1.013228	-1.347262	3.623352
H	4.656998	-0.812813	1.983628
H	5.423734	-0.996962	3.366961

H	1.971359	3.112234	4.254323
H	0.756081	2.417350	3.529095
H	-2.143273	3.065054	0.457789
H	-0.566754	3.059437	0.412537
H	3.699920	4.471159	-2.869698
H	3.292739	3.028484	-2.466418
H	5.309919	2.314245	0.547481
H	4.885353	3.074934	-0.794734
H	5.831885	-0.176755	-2.268000
H	5.199808	0.869271	-1.261873
H	3.744108	0.761186	-2.681978
H	3.007473	1.195389	-3.997058
H	4.613043	-0.985231	-0.246559
H	3.301557	-0.776120	0.539561
H	1.115285	0.243209	0.651878
H	1.982960	0.077085	1.933722
H	5.732796	2.638052	2.846665
H	5.141327	1.208954	2.585387
O	3.489965	4.715087	0.566409
H	3.700063	5.602045	0.870492
H	3.462801	4.739633	-0.404949

$Na^+ (H_2O)_{18}$

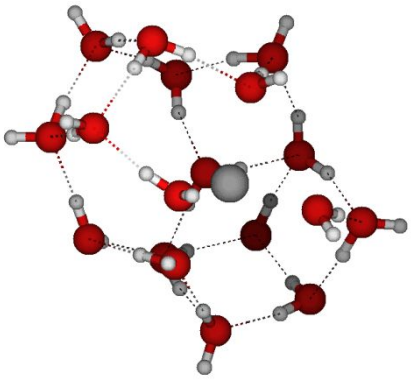


Figure S_{32} : Na^+ optimized structure with 18 water molecules.

E = -1375.047235
H = -1375.046291

O	-0.488367	0.288061	0.311236
O	2.039812	0.849832	1.065236
Na	2.703889	3.100490	1.186708
O	3.129070	4.839757	-0.444542
O	1.239730	2.154965	4.821157
O	0.698696	3.497491	-0.115349
O	-1.050530	1.670121	3.780185
O	0.583961	1.615323	-1.941640
O	4.955160	2.301668	1.708129
O	-1.436759	2.709265	1.221686
O	6.094973	1.985453	-0.808051
O	5.057331	-0.162174	-1.752425
O	4.709592	-0.170921	2.747361
O	3.844130	-1.138340	0.554482
O	3.179825	1.204945	-3.025863
O	2.084462	-0.111181	3.605176
O	-0.405774	-0.907340	2.851228

O	4.416976	3.532137	-2.467977
H	-0.604889	-0.371171	1.021354
H	-1.003317	1.072431	0.599316
H	0.663765	2.840864	-0.872021
H	1.069837	4.317435	-0.470610
H	-1.005438	0.729549	3.518135
H	-1.232462	2.157436	2.951755
H	1.463556	1.332711	-2.252667
H	0.205045	0.877683	-1.434312
H	3.051014	-0.264585	3.541212
H	1.928238	0.666867	4.189007
H	0.529510	-0.858918	3.150899
H	-0.774034	-1.719137	3.215690
H	4.480725	-0.651043	1.875125
H	5.451102	-0.639689	3.145549
H	1.152163	2.241822	5.776614
H	0.300345	2.026988	4.449364
H	-2.270708	3.096601	0.935963
H	-0.708402	3.198072	0.756335
H	4.759863	3.974727	-3.251906
H	3.910872	2.739575	-2.782168
H	5.776446	2.125420	0.109343
H	5.665998	2.674284	-1.349752
H	5.706209	-0.702721	-2.216366
H	5.551339	0.639375	-1.368189
H	3.840097	0.576596	-2.619567
H	3.046595	0.919916	-3.936981
H	4.340921	-0.933094	-0.262414

H	3.092898	-0.503842	0.552724
H	1.128600	0.696802	0.711697
H	1.995851	0.529724	1.997839
H	5.450171	2.871255	2.307753
H	4.932166	1.408977	2.145165
H	3.494829	5.720223	-0.314219
H	3.572614	4.478874	-1.244089
O	2.377150	4.047021	3.257677
H	2.087768	4.928734	3.507513
H	1.983417	3.435692	3.922409

$Na^+ (H_2O)_{19}$

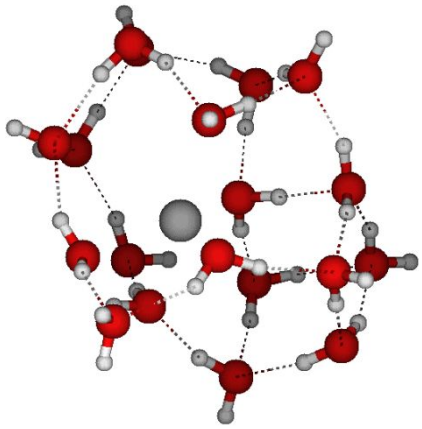


Figure S_{33} : Na^+ optimized structure with 19 water molecules.

E = -1451.420045
H = -1451.419101

O	-0.461022	0.041366	0.312269
O	2.078595	0.677951	0.891788
Na	2.669935	2.928699	0.968519
O	2.666352	4.193106	2.870368

O	2.615017	4.960433	-0.347098
O	0.503135	3.263707	-0.186408
O	4.876267	2.080916	1.690982
O	0.492773	1.401607	-2.045975
O	-1.545059	2.423786	1.190681
O	4.808539	-0.412752	2.623318
O	3.863404	-1.311136	0.425663
O	1.504532	2.366872	4.565099
O	-0.839608	1.659893	3.760165
O	2.262930	-0.027736	3.510494
O	-0.200463	-0.957450	2.940146
O	4.589009	3.489689	-1.712131
O	3.224360	1.434348	-2.870668
O	4.926445	-0.416967	-2.015761
O	6.161820	1.383118	-0.652884
H	-0.511740	-0.581234	1.061684
H	-1.000781	0.812148	0.592760
H	0.481571	2.634208	-0.962243
H	0.902133	4.094876	-0.491578
H	-0.776738	0.703559	3.568011
H	-1.156289	2.058643	2.924641
H	1.423990	1.234555	-2.280883
H	0.186023	0.642429	-1.523624
H	3.213209	-0.263786	3.440184
H	2.165268	0.810824	4.018555
H	0.742823	-0.836551	3.195546
H	-0.508822	-1.753252	3.385882
H	4.557563	-0.852336	1.737336

H	5.557782	-0.893921	2.989096
H	1.468236	2.478680	5.521386
H	0.555072	2.163958	4.269585
H	-2.409708	2.736239	0.905631
H	-0.855257	2.934158	0.685000
H	5.130530	3.932958	-2.374376
H	4.044982	2.823718	-2.202984
H	5.851158	1.441388	0.272892
H	5.778107	2.199223	-1.026073
H	5.495327	-0.933655	-2.597021
H	5.513105	0.220266	-1.491291
H	3.809004	0.656898	-2.650731
H	3.129742	1.446971	-3.829974
H	4.295386	-1.199671	-0.441513
H	3.124789	-0.659561	0.421364
H	1.147965	0.493896	0.605252
H	2.093500	0.439908	1.848906
H	5.305386	2.725893	2.263840
H	4.890605	1.218203	2.177028
H	2.738343	5.759462	0.190269
H	3.393827	4.806941	-0.907137
H	2.329791	5.096884	2.807029
H	2.211383	3.734305	3.605141
O	2.229185	6.885674	1.707878
H	2.798114	7.587125	2.044997
H	1.373300	7.304372	1.559242

$K^+ (H_2O)$

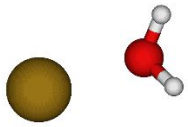


Figure S_{34} : K^+ optimized structure with 1 water molecule.

E = -104.565407
H = -104.564463

K	-0.099939	0.000000	-0.236271
O	0.101647	0.000000	2.398084
H	0.906102	0.000000	2.929567
H	-0.609250	0.000000	3.049574

$K^+ (H_2O)_2$

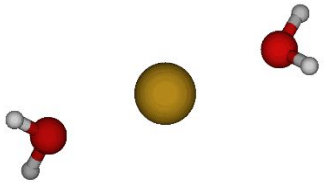


Figure S_{35} : K^+ optimized structure with 2 water molecules.

E = -180.957515
H = -180.956570

O	0.017972	-0.302994	2.871896
K	0.629607	0.666428	0.467144
H	0.596133	-0.757936	3.494736
H	-0.835764	-0.278727	3.318778
O	0.980542	2.166918	-1.706073

H	1.274698	3.083907	-1.748098
H	0.841982	1.922291	-2.628087

$K^+ (H_2O)_3$

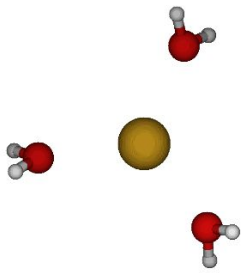


Figure S_{36} : K^+ optimized structure with 3 water molecules.

E = -257.346670
H = -257.345726

O	0.091862	0.049871	2.522424
K	0.911913	0.377853	-0.011047
O	0.472946	2.724434	-1.232437
H	0.624514	-0.175557	3.293129
H	-0.804089	0.128200	2.868327
H	0.772469	3.598500	-0.958916
H	-0.020939	2.886406	-2.043818
O	2.150997	-1.584891	-1.356469
H	1.820626	-2.468283	-1.553917
H	3.028947	-1.566230	-1.753157

$K^+ (H_2O)_4$

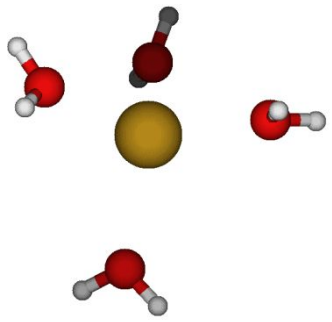


Figure S_{37} : K^+ optimized structure with 4 water molecules.

E = -333.732583
H = -333.731639

O	-0.069197	0.006382	2.143555
K	0.495043	0.354859	-0.483351
O	1.091216	2.938305	-1.040899
O	2.633592	-1.185308	-1.113308
H	-0.078631	-0.816529	2.644109
H	-0.277123	0.684615	2.795169
H	1.953996	3.302472	-1.266313
H	0.496287	3.695093	-1.074443
H	2.724675	-1.776771	-1.868116
H	3.460887	-1.285262	-0.630233
O	-1.649791	-0.341171	-1.984567
H	-2.417169	-0.853190	-1.707424
H	-1.832585	-0.114358	-2.902661

$K^+ (H_2O)_5$

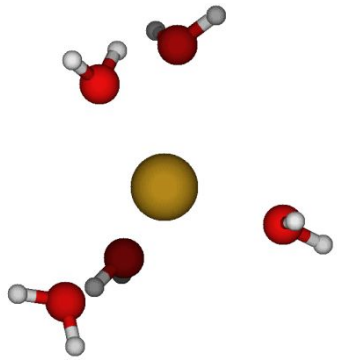


Figure S_{38} : K^+ optimized structure with 5 water molecules.

E = -410.116832
H = -410.115888

O	-0.549768	0.552279	2.159210
K	0.247754	0.627879	-0.426572
O	-1.182639	-0.756502	-2.167386
O	2.349094	2.150864	-0.933630
O	2.983907	-0.545907	-0.660042
H	-0.977442	-0.172939	2.627044
H	-0.463543	1.247758	2.819973
H	2.972428	1.407482	-0.932358
H	2.865604	2.946358	-1.088357
H	3.255419	-1.071960	-1.421271
H	3.534032	-0.860760	0.066558
H	-1.515778	-1.514903	-2.654604
H	-1.712609	0.008418	-2.441514
O	-1.907436	1.927323	-2.029329
H	-1.715401	2.533128	-2.754601
H	-2.775912	2.195101	-1.707209

$K^+ (H_2O)_6$

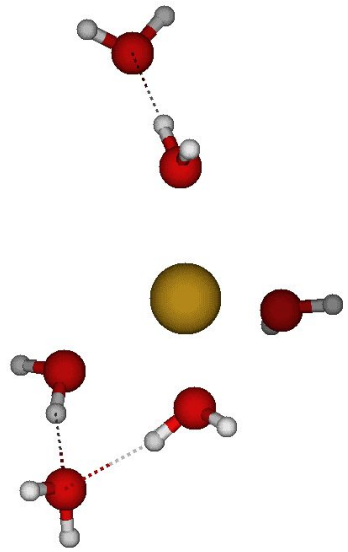


Figure S_{39} : K^+ optimized structure with 6 water molecules.

E = -486.503612
H = -486.502667

O	-1.512073	1.676823	0.996997
K	0.316480	-0.073832	0.093251
O	2.840051	0.722807	0.176581
O	-1.166113	0.286368	-2.119783
O	-3.143933	2.189488	-1.302117
O	4.737809	-0.576514	-1.335083
H	-1.764536	2.121945	1.810735
H	-2.157170	1.960554	0.328313
H	3.547150	0.292851	-0.346490
H	3.268514	1.458491	0.622746
H	5.167459	-0.135735	-2.075522
H	5.429810	-1.088637	-0.903734
H	-1.151569	0.065307	-3.055178
H	-1.894686	0.919568	-2.008582

H	-3.133244	3.073239	-1.688433
H	-4.070137	1.920377	-1.290761
O	-0.045821	-2.584101	1.074974
H	0.111533	-2.897855	1.971607
H	-0.403257	-3.348262	0.610864

$K^+ (H_2O)_7$

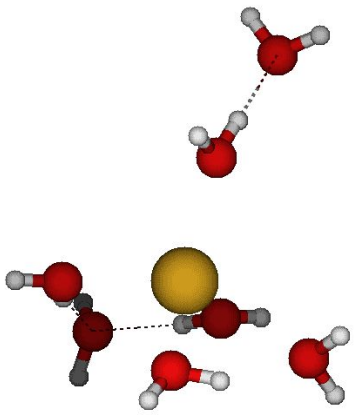


Figure S_{40} : K^+ optimized structure with 7 water molecules.

E = -562.884714
H = -562.883769

O	-1.111647	2.657634	0.276762
K	0.032228	0.231944	0.632616
O	2.700223	0.342335	0.579944
O	-1.404269	-0.122623	-1.641469
O	-0.143150	-2.791686	1.465736
O	4.184627	0.310615	-1.752047
O	-2.829797	2.343856	-1.998645
H	-1.224757	3.457051	0.798324
H	-1.737557	2.730758	-0.461534
H	3.244932	0.328143	-0.232409

H	3.294158	0.643571	1.273253
H	4.577632	1.127690	-2.076044
H	4.854656	-0.367543	-1.887131
H	-1.406343	-0.698540	-2.411048
H	-1.943542	0.646696	-1.889027
H	-2.682179	2.887892	-2.781034
H	-3.784440	2.334741	-1.862100
H	0.639351	-3.315875	1.670003
H	-0.798733	-3.427128	1.157518
O	-0.799229	-0.602917	3.025807
H	-0.696544	-1.545519	2.816866
H	-1.176672	-0.550837	3.907538

$K^+ (H_2O)_8$

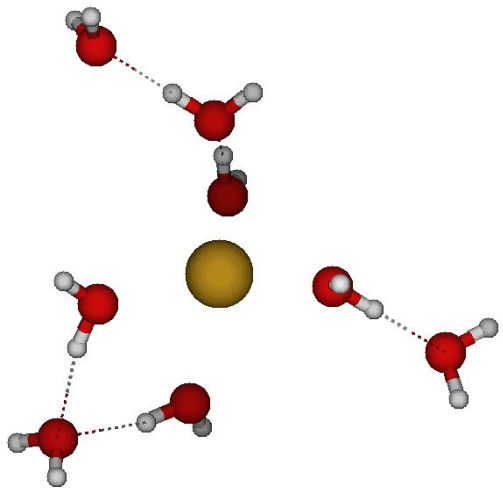


Figure S_{41} : K^+ optimized structure with 8 water molecules.

E = -639.267678
H = -639.266734

O	-0.482720	2.433746	-0.563258

K	0.043369	-0.187904	-0.110156
O	-0.187934	-0.998387	2.431006
O	2.997078	-0.117018	-0.142907
O	-2.451712	-0.248971	-1.197150
O	4.469588	1.980239	-1.117047
O	-1.502483	-3.392468	2.859927
O	-3.072400	2.492353	-1.804934
H	-0.029591	3.280103	-0.520852
H	-1.334242	2.610813	-0.994940
H	3.536515	0.630845	-0.478900
H	3.533584	-0.542258	0.533378
H	5.040620	2.513997	-0.554902
H	4.955698	1.859625	-1.939446
H	-2.934640	-0.910391	-1.700375
H	-2.804497	0.609313	-1.481240
H	-3.168382	2.786360	-2.718137
H	-3.805153	2.891787	-1.321867
H	-1.040828	-4.146402	3.240896
H	-2.391317	-3.420214	3.228364
H	-0.649187	-1.837975	2.627051
H	-0.121597	-0.543767	3.275015
O	1.492611	-1.665864	-1.802426
H	1.790183	-2.360354	-2.394782
H	2.287972	-1.271420	-1.398929

$K^+ (H_2O)_9$

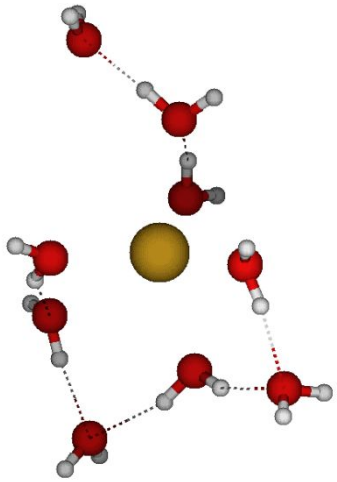


Figure S_{42} : K^+ optimized structure with 9 water molecules.

E = -715.651525
H = -715.650581

O	-0.903066	2.445011	-1.012694
K	0.488720	0.036511	0.154705
O	1.682521	-0.545207	-2.222707
O	0.228973	-1.834646	2.136060
O	-2.114695	-0.730222	-0.099595
O	3.413581	-0.393011	-0.119334
O	5.169763	1.700455	-0.202090
O	-2.512374	-2.700262	1.991880
O	-3.597366	1.561996	-1.155394
H	-0.626465	2.853810	-1.838084
H	-1.846473	2.225141	-1.114294
H	4.057743	0.347465	-0.127819
H	3.899165	-1.157985	0.204271
H	5.679985	2.004627	0.555135
H	5.732918	1.837221	-0.970628
H	-2.483697	-1.302651	0.588058

H	-2.791801	-0.075539	-0.318614
H	-3.966265	1.350143	-2.020791
H	-4.265503	2.095632	-0.709974
H	-2.602457	-3.580491	1.608566
H	-3.104718	-2.685135	2.752015
H	-0.678487	-2.177101	2.192950
H	0.577166	-1.881172	3.030878
H	1.750592	-1.218079	-2.905048
H	2.503738	-0.597950	-1.697412
O	0.365670	2.427291	1.404335
H	0.640309	3.189758	1.919389
H	-0.121923	2.770369	0.634200

$K^+ (H_2O)_{10}$

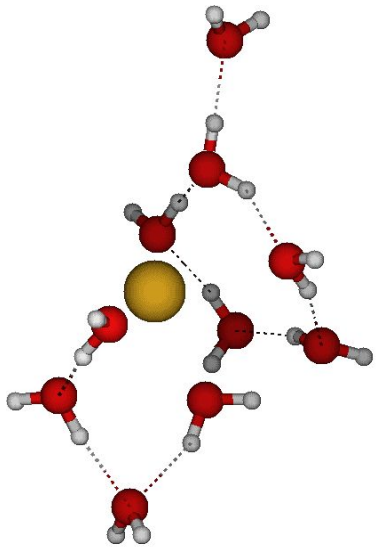


Figure S_{43} : K^+ optimized structure with 10 water molecules.

E = -792.051742
H = -792.050798

O	-1.856640	2.827666	-1.231115
O	-0.311596	3.440278	0.947000
K	0.339313	1.090856	-0.103252
O	1.487307	-0.756583	-1.940110
O	-1.987006	-0.403291	-0.123209
O	2.903379	-0.171261	0.182554
O	5.617133	-0.497179	0.394309
O	0.982153	-0.769285	1.991851
O	-4.214558	1.331123	-0.627611
O	-0.849364	-2.544742	1.210995
H	-1.964744	3.352262	-2.030675
H	-2.713721	2.389967	-1.077208
H	3.870289	-0.286367	0.284654

H	2.460747	-0.570625	0.958007
H	6.188956	0.184006	0.761802
H	6.044774	-1.335464	0.595247
H	-1.972923	-1.085648	0.571107
H	-2.873673	-0.013440	-0.157513
H	-4.809807	1.059445	-1.336466
H	-4.783038	1.677136	0.070647
H	-0.641502	-2.691693	0.235905
H	-1.071356	-3.401245	1.589789
H	0.366579	-1.526269	1.827743
H	1.031318	-0.657559	2.945808
H	1.945268	-0.830714	-2.782890
H	2.183462	-0.689394	-1.233231
H	-0.196963	4.276872	1.404480
H	-0.993157	3.576764	0.265704
O	-0.557766	-2.484278	-1.360592
H	-1.238361	-1.790595	-1.376660
H	0.257932	-2.010634	-1.635121

$K^+ (H_2O)_{11*}$

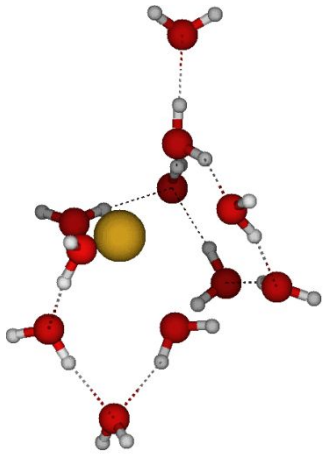


Figure S_{44} : K^+ optimized structure with 11 water molecules.

E = -868.437512
H = -868.436568

O	-2.016625	3.179928	-0.709270
O	-0.241407	3.463765	1.351731
K	0.367756	1.363462	-0.181006
O	-1.847354	-0.300468	-0.307657
O	-0.893291	-2.443897	1.146907
O	-0.498764	-2.527818	-1.400474
O	0.907931	-0.651692	1.945297
O	2.752635	-0.253650	0.049789
O	1.934607	-1.439896	-2.133598
O	5.471057	-0.213882	0.453794
O	-4.195889	1.339466	-0.646426
H	-2.126051	3.806417	-1.431134
H	-2.826128	2.639050	-0.694513
H	3.711974	-0.216486	0.241600
H	2.286667	-0.558825	0.858303
H	5.963689	0.612329	0.487394
H	5.933632	-0.816418	1.044810
H	-1.864818	-0.966723	0.402802
H	-2.737582	0.076477	-0.383475
H	-4.695234	1.182368	-1.456698
H	-4.855045	1.434092	0.051362
H	-0.652700	-2.648019	0.188558
H	-1.190111	-3.263683	1.553823
H	0.282141	-1.399811	1.778322

H	0.994675	-0.569953	2.899479
H	2.589804	-1.984831	-2.581192
H	2.354609	-1.087611	-1.296867
H	-0.166183	4.188146	1.977646
H	-1.021372	3.647105	0.798609
H	-1.060414	-1.739025	-1.487285
H	0.388104	-2.245290	-1.710846
O	1.013185	1.078261	-2.786238
H	1.389353	0.176332	-2.807183
H	1.344347	1.521352	-3.571585

$K^+ (H_2O)_{12}$

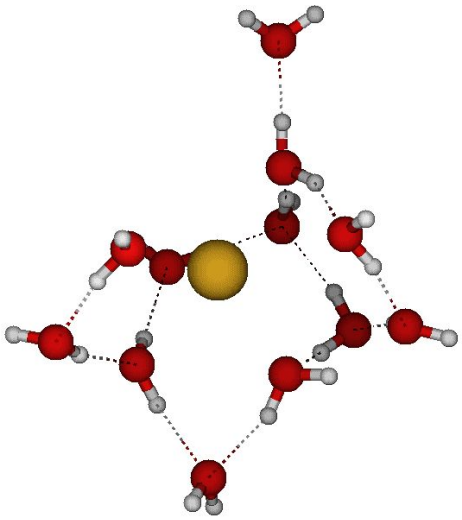


Figure S_{45} : K^+ optimized structure with 12 water molecules.

E = -944.825975
H = -944.825031

O	-1.495070	2.564605	-1.243389
O	-1.018347	4.903445	0.061212
K	0.559026	1.315126	0.386017

O	0.609908	1.396572	-2.543560
O	1.490371	-1.171791	-2.357819
O	2.754189	-0.422659	-0.205484
O	1.323226	-1.041779	1.978452
O	-0.677617	-2.665946	1.303967
O	-0.751494	-2.426485	-1.276289
O	5.489524	-0.327140	-0.247222
O	-1.699209	-0.305663	0.276180
O	-3.938622	1.151537	-0.623844
H	-0.941303	2.149230	-1.931671
H	-2.350796	2.108733	-1.224967
H	3.733288	-0.387770	-0.178957
H	2.436885	-0.840891	0.625031
H	5.971377	0.483254	-0.053381
H	6.060714	-1.046004	0.041488
H	-1.738639	-1.045026	0.906825
H	-2.594723	0.050242	0.151036
H	-4.545766	0.778736	-1.273603
H	-4.476434	1.720716	-0.060735
H	-0.612513	-2.769506	0.306371
H	-0.919244	-3.522124	1.670762
H	0.628469	-1.732299	1.826532
H	1.659520	-1.184001	2.868430
H	2.024452	-1.624493	-3.019029
H	2.078461	-0.983608	-1.568277
H	-0.835010	5.643516	-0.525430
H	-1.266741	4.150875	-0.517389
H	-1.226239	-1.597633	-1.082264

H	0.066719	-2.133561	-1.725426
H	0.878160	0.458190	-2.667027
H	1.139171	1.910252	-3.160934
O	0.991636	3.711835	1.396285
H	1.217977	4.163116	2.213570
H	0.307110	4.276553	0.963205

$K^+ (H_2O)_{13}$

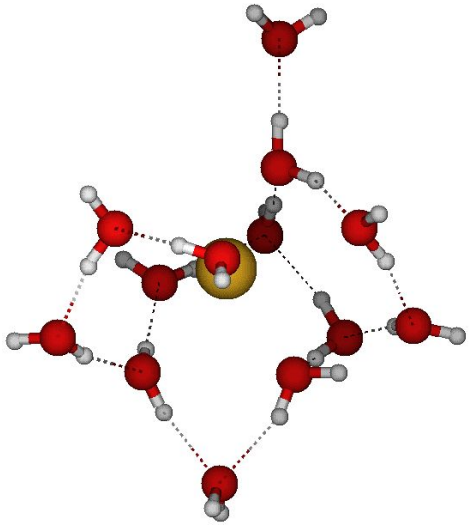


Figure S_{46} : K^+ optimized structure with 13 water molecules.

E = -1021.210956
H = -1021.210012

O	-1.558928	2.575347	-0.951923
O	-0.911082	5.010937	-0.021217
O	1.368850	4.031431	0.895319
K	0.565027	1.281845	0.592063
O	0.473204	1.469254	-2.383070
O	1.514640	-1.032728	-2.370141
O	2.813358	-0.371966	-0.215799
O	1.387428	-1.271570	1.845297
O	-0.633051	-2.857424	1.129834
O	-0.714676	-2.412298	-1.424544
O	5.556620	-0.465044	-0.273825
O	-1.649292	-0.418127	0.291689
O	-3.957481	1.056012	-0.417217
H	-1.020518	2.158813	-1.653924

H	-2.412538	2.116263	-0.912318
H	3.792881	-0.391210	-0.202780
H	2.489217	-0.868444	0.569351
H	6.087879	0.259730	0.071366
H	6.034515	-1.268364	-0.043405
H	-1.653452	-1.199329	0.871866
H	-2.555539	-0.075747	0.225324
H	-4.534075	0.723333	-1.114826
H	-4.536054	1.513910	0.203661
H	-0.576600	-2.885813	0.127012
H	-0.867759	-3.739393	1.434418
H	0.698056	-1.961086	1.679025
H	1.624284	-1.325707	2.775614
H	2.058283	-1.397491	-3.076193
H	2.112877	-0.862012	-1.581242
H	-0.946152	5.695186	-0.696379
H	-1.263057	4.190720	-0.438281
H	-1.185565	-1.601201	-1.157812
H	0.111623	-2.080386	-1.829236
H	0.791427	0.551572	-2.545181
H	0.993288	2.037300	-2.958886
H	2.090076	4.666544	0.929158
H	0.573439	4.521608	0.552698
O	0.598605	2.502178	2.998802
H	0.909366	3.267831	2.473887
H	0.095569	2.864819	3.732591

$K^+ (H_2O)_{14}$

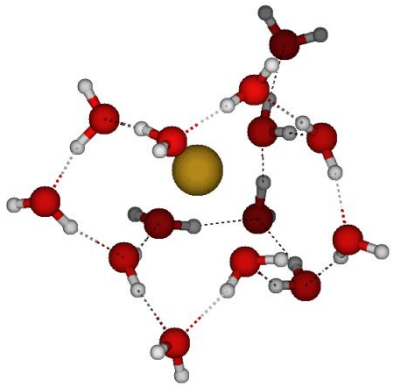


Figure S_{47} : K^+ optimized structure with 14 water molecules.

E = -1097.599949
H = -1097.599005

O	-1.399901	2.565818	-1.012053
O	-0.833599	5.006468	-0.097081
O	1.248233	4.030047	1.146328
O	0.088716	2.562189	3.021519
K	0.770145	1.286682	0.499061
O	0.557962	1.487361	-2.514911
O	1.369969	-1.078054	-2.522152
O	2.755816	-0.466576	-0.442413
O	1.859851	-1.606158	1.717813
O	-0.584174	-2.758275	1.215166
O	-0.822268	-2.332358	-1.353727
O	5.484931	-0.757423	-0.689933
O	-1.479626	-0.302899	0.463653
O	-3.797084	1.064036	-0.414794
H	-0.873647	2.166216	-1.736196
H	-2.249202	2.099638	-0.958451

H	3.732097	-0.519622	-0.509548
H	2.490030	-1.009263	0.356128
H	6.073873	-0.080379	-0.340546
H	5.816731	-1.589469	-0.335474
H	-1.479425	-1.113980	1.007026
H	-2.387470	0.033775	0.399044
H	-4.314549	0.618076	-1.095432
H	-4.433496	1.560732	0.112384
H	-0.580988	-2.823356	0.216846
H	-0.870488	-3.610386	1.558755
H	1.004886	-2.081690	1.658534
H	1.783719	-0.912989	2.403061
H	1.867976	-1.488733	-3.236614
H	2.005299	-0.928846	-1.749265
H	-0.769266	5.663697	-0.796599
H	-1.156930	4.174691	-0.520699
H	-1.184909	-1.487326	-1.031603
H	-0.019246	-2.064944	-1.844155
H	0.795898	0.542286	-2.676739
H	1.017613	1.998534	-3.187222
H	1.951772	4.663734	1.316657
H	0.521623	4.520796	0.663356
H	0.509650	3.293327	2.506696
H	-0.559708	2.953880	3.612965
O	1.942551	0.653312	3.308437
H	2.304911	0.457790	4.177661
H	1.240398	1.328442	3.440892

Mg^{2+} (H_2O)

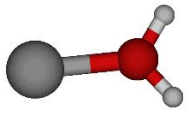


Figure S_{48} : Mg^{2+} optimized structure with 1 water molecule.

E = -275.689796
H = -275.688852

Mg	-0.096933	0.000000	0.172252
O	0.093237	0.000000	2.102208
H	0.928235	0.000000	2.614091
H	-0.625979	0.000000	2.767002

Mg^{2+} $(H_2O)_2$

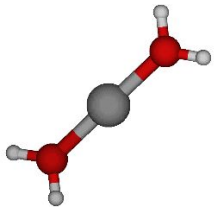


Figure S_{49} : Mg^{2+} optimized structure with 2 water molecules.

E = -352.241551
H = -352.240607

O	0.235421	0.000003	2.372084
Mg	-1.024035	-0.000002	0.870809
H	1.208446	-0.000916	2.323656
H	0.018298	0.000931	3.321844
O	-2.283637	-0.000007	-0.630247
H	-2.066538	0.002410	-1.580021

H -3.256678 -0.002420 -0.581820

Mg^{2+} $(H_2O)_3$

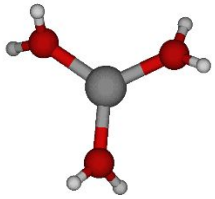


Figure S_{50} : Mg^{2+} optimized structure with 3 water molecules.

E = -428.729600
H = -428.728656

O	-0.005330	0.000782	2.053612
Mg	-0.830643	0.000640	0.247005
O	0.321185	0.007267	-1.371792
O	-2.808112	-0.009567	0.057729
H	0.782651	-0.490848	2.336666
H	-0.307685	0.491798	2.834802
H	0.185589	-0.501133	-2.187809
H	1.134633	0.519367	-1.508981
H	-3.336139	0.490161	-0.585841
H	-3.444342	-0.515047	0.589163

Mg^{2+} $(H_2O)_4$

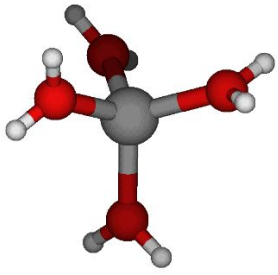


Figure S_{51} : Mg^{2+} optimized structure with 4 water molecules.

E = -505.200068

H = -505.199124

O	0.066778	-0.420516	1.981702
Mg	-0.527978	0.484285	0.278092
O	-2.522778	0.297368	0.030593
O	0.366033	-0.363578	-1.320964
H	0.523849	-1.271096	2.052723
H	-0.029251	-0.090946	2.886869
H	0.148644	-1.210160	-1.737174
H	1.094576	0.010252	-1.837607
H	-3.027536	0.426026	-0.785375
H	-3.166328	0.041190	0.707078
O	-0.020764	2.433821	0.413654
H	0.810664	2.804231	0.743371
H	-0.576140	3.190273	0.175350

Mg^{2+} $(H_2O)_5$

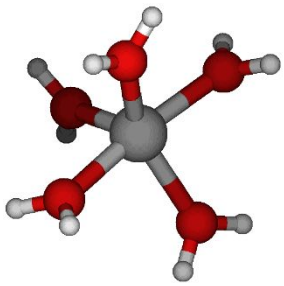


Figure S_{52} : Mg^{2+} optimized structure with 5 water molecules.

E = -581.644672
H = -581.643728

O	0.481386	-0.854822	1.673525
Mg	-0.839745	0.293184	0.610610

O	-0.299248	2.278605	0.686681
O	-2.538293	0.051393	-0.506844
O	0.276741	-0.132515	-1.112492
H	1.291049	-1.259337	1.338094
H	0.425953	-1.076749	2.611293
H	0.369387	-0.969047	-1.585914
H	0.814954	0.510629	-1.591120
H	-2.583462	-0.098292	-1.459350
H	-3.448042	0.089065	-0.186435
H	0.461300	2.653975	1.149706
H	-0.754941	3.018944	0.264817
O	-2.050351	0.372220	2.320342
H	-2.195614	1.164325	2.853143
H	-2.564080	-0.331855	2.736115

Mg^{2+} $(H_2O)_6$

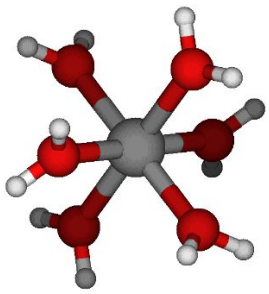


Figure S_{53} : Mg^{2+} optimized structure with 6 water molecules.

E = -658.083768
H = -658.082824

O	0.922975	-0.391707	1.665934
Mg	-0.761991	-0.000468	0.467629
O	-1.984814	-0.041067	2.182044

O	-0.453505	2.065353	0.736424
O	-2.447475	0.394393	-0.731818
O	0.458089	0.039952	-1.246530
H	1.832025	-0.487691	1.360124
H	0.930042	-0.540758	2.618244
H	0.684541	-0.708398	-1.810239
H	0.903257	0.812478	-1.613111
H	-2.453037	0.520694	-1.687364
H	-3.356312	0.503140	-0.429209
H	0.248376	2.467474	1.260656
H	-0.977239	2.785864	0.368226
H	-2.207668	0.705559	2.749454
H	-2.437059	-0.812400	2.542097
O	-1.071892	-2.067293	0.199378
H	-1.777202	-2.474956	-0.315895
H	-0.537028	-2.783487	0.559797

Mg^{2+} $(H_2O)_7$

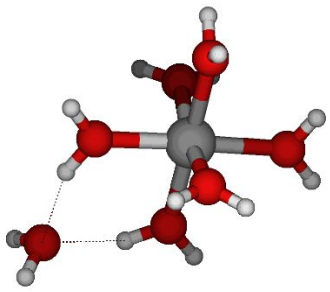


Figure S_{54} : Mg^{2+} optimized structure with 7 water molecules.

E = -734.513070
H = -734.512126

O	1.106837	-0.673579	1.600895

Mg	-0.680451	-0.242042	0.565837
O	-0.825557	-2.309635	0.126919
O	-1.604892	-0.610031	2.441514
O	-0.607459	1.802556	0.959816
O	-2.441446	0.222787	-0.454627
O	0.599885	-0.014108	-1.112143
H	1.997194	-0.619379	1.237538
H	1.185830	-0.837476	2.546735
H	0.736695	-0.668840	-1.805188
H	0.886901	0.832594	-1.469972
H	-3.074457	-0.316209	-0.936641
H	-2.751945	1.152244	-0.489725
H	0.050522	2.305570	1.448546
H	-1.299587	2.418358	0.636954
H	-1.910434	0.076138	3.044105
H	-2.052945	-1.423514	2.696827
H	-1.475458	-2.825909	-0.361634
H	-0.155929	-2.929785	0.436892
O	-2.796452	2.928132	-0.206487
H	-3.523813	3.284282	0.319243
H	-2.717966	3.511392	-0.971945

Mg^{2+} $(H_2O)_8$

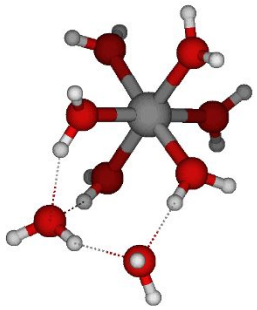


Figure S_{55} : Mg^{2+} optimized structure with 8 water molecules.

E = -810.938972
H = -810.938028

O	1.169981	-0.649274	1.640602
Mg	-0.416626	-0.300401	0.299827
O	1.042523	-0.157893	-1.224855
O	-0.568858	-2.384860	-0.023325
O	-1.706683	-0.458091	1.956925
O	-0.342141	1.771966	0.484833
O	-2.037234	0.009313	-0.985323
O	-2.919651	2.350973	0.040084
H	2.112111	-0.632132	1.442912
H	1.074522	-0.684176	2.598136
H	1.386337	-0.840829	-1.809743
H	1.317059	0.692164	-1.585328
H	-2.100943	-0.158971	-1.929739
H	-2.568817	0.811311	-0.785509
H	0.242528	2.330860	1.003723
H	-1.178512	2.257945	0.308803
H	-2.379163	0.200166	2.230533
H	-2.017254	-1.316216	2.261017

H	-1.278053	-2.831676	-0.497590
H	0.029539	-3.065320	0.302683
H	-3.387982	2.204960	0.886354
H	-3.343842	3.085408	-0.417808
O	-3.726096	1.406685	2.518273
H	-3.626724	1.979129	3.289431
H	-4.615157	1.036320	2.587467

Mg^{2+} $(H_2O)_9$

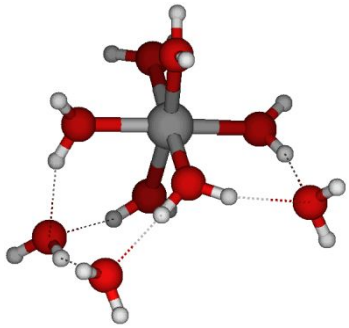


Figure S_{56} : Mg^{2+} optimized structure with 9 water molecules.

E = -887.363901
H = -887.362957

O	1.282881	-0.344659	1.547302
Mg	-0.312424	-0.200300	0.160583
O	-1.902893	0.260938	-1.116025
O	1.196782	0.187767	-1.285419
O	-0.389196	-2.232421	-0.310821
O	-1.607904	-0.618887	1.755867
O	-0.286549	1.865904	0.489449
O	-2.827696	2.530925	0.007257
O	-3.700362	1.267288	2.327636
H	2.221565	-0.376419	1.338706
H	1.179512	-0.569896	2.476729
H	1.571417	-0.318725	-2.012477
H	1.309603	1.119158	-1.505912
H	-2.211932	-0.172570	-1.914730
H	-2.420853	1.077929	-0.962554
H	0.247665	2.324273	1.143367
H	-1.111141	2.376148	0.329404

H	-2.329568	-0.015445	2.013561
H	-1.921120	-1.534245	1.869662
H	0.195900	-2.788648	-0.831287
H	-0.954139	-2.816872	0.238226
H	-3.316814	2.264369	0.810723
H	-3.240061	3.321626	-0.356773
H	-3.601822	1.750219	3.157363
H	-4.602888	0.926192	2.338439
H	-2.892008	-3.766441	1.225767
O	-2.053086	-3.386626	1.512524
H	-1.705753	-3.992432	2.178170

Mg^{2+} $(H_2O)_{10}$

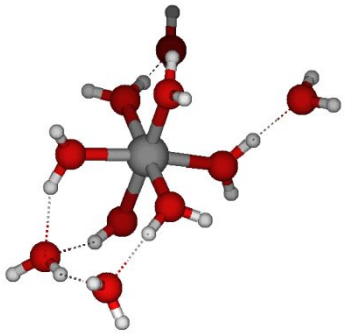


Figure S_{57} : Mg^{2+} optimized structure with 10 water molecules.

E = -963.782903
H = -963.781958

O	1.046521	-0.385676	1.608796
Mg	-0.585304	-0.184304	0.291642
O	-0.520825	1.909331	0.491308
O	-2.314992	0.162512	-0.869912
O	0.740716	-0.000642	-1.282928

O	-0.866816	-2.226933	0.104887
O	-1.796296	-0.313608	2.033998
O	0.816927	-4.190758	0.558398
O	-3.139418	2.498911	0.261661
O	-3.802988	1.542681	2.775305
H	1.961509	-0.545216	1.360434
H	0.964594	-0.536334	2.555036
H	1.158413	-0.647661	-1.909009
H	0.966733	0.882873	-1.585726
H	-2.356228	0.083993	-1.826915
H	-2.825735	0.960258	-0.615540
H	0.083875	2.422884	1.032736
H	-1.366076	2.397783	0.400412
H	-2.455315	0.323882	2.370185
H	-2.128277	-1.196209	2.223910
H	-1.596198	-2.589491	-0.404240
H	-0.222942	-2.966099	0.271732
H	-3.544754	2.333657	1.136110
H	-3.600016	3.238589	-0.148576
H	-3.646851	2.101808	3.546102
H	-4.684698	1.171289	2.901156
H	0.709655	-4.836606	1.262693
H	1.345498	-4.615983	-0.122611
O	1.911498	-1.659115	-2.969182
H	2.868734	-1.710374	-3.046828
H	1.559927	-1.883557	-3.835626

Mg^{2+} $(H_2O)_{11}$

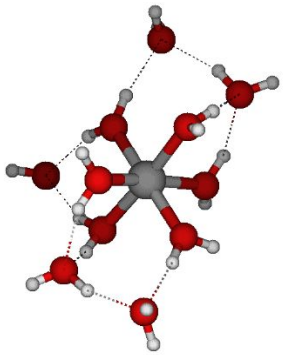


Figure S_{58} : Mg^{2+} optimized structure with 11 water molecules.

E = -1040.209120
H = -1040.208176

O	0.870003	-0.913139	1.411274
Mg	-0.807977	-0.237064	0.360552
O	-2.086676	-0.434209	2.025134
O	-0.433130	1.721005	0.994566
O	-2.390167	0.495514	-0.792129
O	0.339372	-0.198230	-1.392306
O	-1.266464	-2.293423	0.093223
O	1.251416	-3.306700	0.249055
O	2.541715	-1.992498	-1.818061
O	-2.934418	2.706505	0.808433
O	-3.746412	1.528108	3.180624
H	1.175079	-1.827407	1.234804
H	1.021667	-0.707046	2.337148
H	1.135804	-0.720549	-1.588841
H	-0.061386	0.104429	-2.226131
H	-2.242679	0.681099	-1.736811
H	-2.829696	1.269635	-0.392096

H	0.388251	2.215335	0.948586
H	-1.193403	2.338205	0.956441
H	-2.635447	0.206411	2.514365
H	-2.454307	-1.311953	2.160166
H	-1.940659	-2.647026	-0.492640
H	-0.492661	-2.894665	0.083090
H	-3.363584	2.455305	1.650476
H	-3.280193	3.566997	0.550970
H	-3.462037	1.936438	4.006914
H	-4.672211	1.290856	3.310871
H	1.556621	-4.158618	0.577465
H	1.802207	-3.057269	-0.519978
H	3.413135	-1.645882	-1.592490
H	2.640441	-2.392056	-2.690142
O	-1.361567	0.777912	-3.384662
H	-1.193727	1.640759	-3.779713
H	-1.736044	0.237027	-4.088928

Mg^{2+} $(H_2O)_{12}$

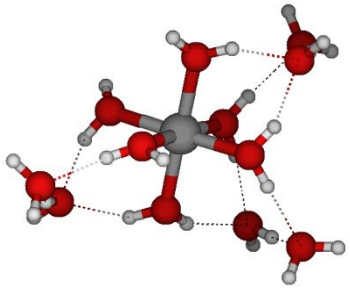


Figure S_{59} : Mg^{2+} optimized structure with 12 water molecules.

E = -1116.627456

H = -1116.626512

O	0.877808	-0.907885	1.502957
Mg	-0.798098	-0.195309	0.474288
O	-1.293996	-2.205255	0.042204
O	-2.001825	-0.403442	2.194464
O	-0.359677	1.752268	1.110326
O	-2.421519	0.546467	-0.605328
O	0.341536	-0.101821	-1.286015
O	1.283232	-3.230804	0.234572
O	-2.797716	2.861369	0.863214
O	2.695362	-1.730817	-1.619082
O	-3.560416	1.702549	3.273567
O	-1.709304	-0.224397	-3.107042
H	1.169891	-1.818818	1.288115
H	0.978396	-0.760609	2.447010
H	1.182964	-0.559420	-1.450161
H	-0.184548	-0.103514	-2.108926
H	-2.354887	0.527286	-1.578870
H	-2.764124	1.409118	-0.306952
H	0.471064	2.196964	0.924720
H	-1.092653	2.397683	1.022746
H	-2.531702	0.280616	2.644224
H	-2.466863	-1.241181	2.272483
H	-1.842801	-2.435512	-0.727933
H	-0.517050	-2.795973	0.046894
H	-3.220316	2.628754	1.713019
H	-3.096039	3.741719	0.614282

H	-3.209197	2.112894	4.072723
H	-4.487876	1.517303	3.461987
H	1.599585	-4.089906	0.531221
H	1.872855	-2.917768	-0.479877
H	3.499448	-1.337666	-1.260160
H	2.927783	-2.027032	-2.506529
H	-1.824358	0.141829	-3.989092
H	-2.110341	-1.114725	-3.089047
O	-2.795336	-2.683437	-2.371663
H	-2.634998	-3.506901	-2.846696
H	-3.749168	-2.647045	-2.235129

Mg^{2+} $(H_2O)_{13}$

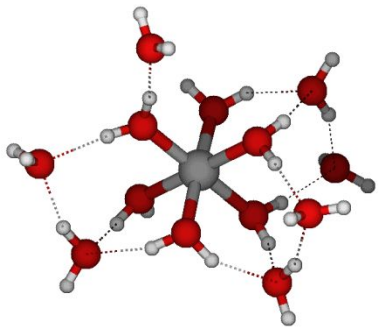


Figure S_{60} : Mg^{2+} optimized structure with 13 water molecules.

E = -1193.040638
H = -1193.039694

O	0.856407	-0.983944	1.454110
Mg	-0.829916	-0.265815	0.439375
O	0.380933	-0.038186	-1.287637
O	-1.257983	-2.240365	-0.166584

O	-1.971774	-0.434202	2.164382
O	-0.400610	1.714427	1.047083
O	-2.430451	0.502681	-0.679756
O	1.337750	-3.230069	0.056976
O	-2.833893	2.835316	0.740530
O	-1.592497	-0.106553	-3.199375
O	2.791960	-1.595748	-1.636704
O	-3.519210	1.802274	3.187816
O	-2.728319	-2.578692	-2.634545
H	1.162965	-1.879903	1.204060
H	0.882594	-0.898402	2.410694
H	1.234998	-0.471978	-1.445258
H	-0.118216	-0.018345	-2.126441
H	-2.311174	0.537784	-1.646608
H	-2.782494	1.355845	-0.362540
H	0.420929	2.137738	0.786060
H	-1.131811	2.355961	0.927589
H	-2.468834	0.292755	2.571878
H	-2.362929	-1.269194	2.504369
H	-1.794599	-2.425285	-0.955778
H	-0.472537	-2.816541	-0.186111
H	-3.236190	2.626504	1.607986
H	-3.138911	3.706914	0.471341
H	-3.151277	2.248478	3.958859
H	-4.430566	1.588504	3.417231
H	1.664544	-4.100379	0.304065
H	1.945311	-2.855531	-0.611324
H	3.567776	-1.205114	-1.218383

H	3.067775	-1.824546	-2.531344
H	-1.680902	0.307373	-4.062969
H	-1.995603	-0.995162	-3.241398
H	-2.589764	-3.380693	-3.150678
H	-3.681335	-2.515368	-2.503682
O	-3.114510	-2.579750	3.310015
H	-3.734163	-3.205909	2.928439
H	-2.879581	-2.922854	4.176114

Mg^{2+} $(H_2O)_{14}$

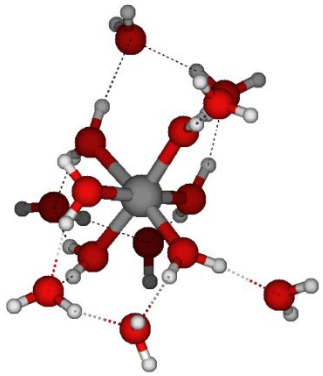


Figure S_{61} : Mg^{2+} optimized structure with 14 water molecules.

E = -1269.453504
H = -1269.452560

O	0.712838	-0.943827	1.476179
Mg	-0.948572	-0.245714	0.472267
O	-2.512286	0.457097	-0.774682
O	0.319201	0.055776	-1.237982
O	-1.295330	-2.218306	-0.175316
O	-2.256422	-0.359510	2.069953
O	-0.552210	1.767542	1.002642
O	-3.475336	-2.465674	3.213506
O	1.244856	-3.239201	0.054659
O	-3.016530	2.823913	0.583447
O	-1.543152	-0.133315	-3.256848
O	-3.869514	1.866476	3.009379
O	2.731042	-1.544519	-1.560063
O	-2.684802	-2.597484	-2.698201
H	1.035853	-1.834377	1.259482
H	1.014188	-0.705815	2.380794

H	1.165012	-0.408368	-1.343433
H	-0.145302	0.033473	-2.095686
H	-2.334235	0.500375	-1.731732
H	-2.897595	1.303248	-0.482041
H	0.222082	2.155889	0.586701
H	-1.307184	2.374299	0.857761
H	-2.739434	0.378744	2.470162
H	-2.650197	-1.186566	2.423264
H	-1.802664	-2.412470	-0.979542
H	-0.499202	-2.784047	-0.167430
H	-3.469402	2.634644	1.430136
H	-3.313276	3.684827	0.274418
H	-3.585368	2.337935	3.800102
H	-4.784550	1.610004	3.168012
H	1.570548	-4.114068	0.283910
H	1.865770	-2.839539	-0.583893
H	3.499908	-1.170856	-1.115315
H	3.019739	-1.738213	-2.458621
H	-1.607750	0.260600	-4.131477
H	-1.926125	-1.030801	-3.294503
H	-2.542009	-3.413949	-3.189536
H	-3.639356	-2.520960	-2.589999
H	-4.062704	-3.092548	2.784822
H	-3.206359	-2.869970	4.042032
O	1.701221	-0.382920	3.903371
H	2.353717	0.298210	4.082899
H	1.445857	-0.747755	4.753695

Mg^{2+} $(H_2O)_{15}$

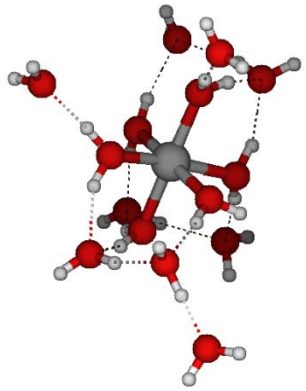


Figure S_{62} : Mg^{2+} optimized structure with 15 water molecules.

E = -1345.871105
H = -1345.870161

O	1.168063	-0.910206	1.133455
Mg	-0.636130	-0.374667	0.277453
O	-0.563037	1.592821	0.883548
O	-2.426756	0.039303	-0.774621
O	0.358656	-0.136742	-1.573242
O	-0.923785	-2.453700	-0.183730
O	-1.796551	-0.851364	1.974555
O	2.017528	-0.530743	3.649200
O	-6.031007	-0.016306	3.859401
O	-3.248705	2.152615	0.734953
O	-1.686509	-0.511837	-3.356125
O	-3.655661	0.867201	3.079578
O	1.707048	-3.244039	-0.228073
O	-2.487452	-3.049690	-2.571656
O	2.895439	-1.473111	-2.001642
H	1.507253	-1.794818	0.915836

H	1.431205	-0.703839	2.057380
H	1.239554	-0.497729	-1.758160
H	-0.189365	-0.212892	-2.376599
H	-2.365392	0.111261	-1.742928
H	-2.901391	0.815723	-0.415249
H	0.168683	2.235123	0.759349
H	-1.409596	2.071963	0.841842
H	-2.461339	-0.287903	2.422972
H	-2.140760	-1.747095	1.926627
H	-1.466066	-2.696322	-0.951728
H	-0.080665	-2.943144	-0.246682
H	-3.549294	1.787595	1.597979
H	-3.771610	2.934256	0.538848
H	-3.311793	1.342416	3.842356
H	-4.544187	0.520483	3.350014
H	2.135965	-4.072147	0.004620
H	2.225035	-2.818626	-0.937489
H	3.616541	-0.989306	-1.584168
H	3.190780	-1.662079	-2.898873
H	-1.882447	-0.167982	-4.231973
H	-1.982827	-1.440973	-3.315920
H	-2.305053	-3.872797	-3.037951
H	-3.426302	-3.073864	-2.356147
H	-6.860252	0.452788	3.736465
H	-6.192255	-0.688288	4.526557
H	2.790786	-0.036531	3.930775
H	1.600621	-0.868511	4.444921
O	1.355079	3.452818	0.557612

H	1.734450	3.978217	1.266067
H	1.551847	3.914313	-0.260805

Mg^{2+} $(H_2O)_{16}$

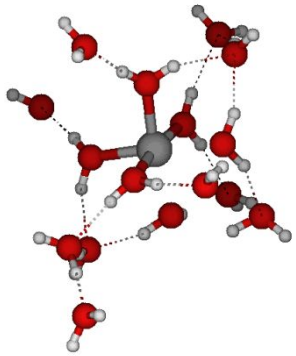


Figure S_{63} : Mg^{2+} optimized structure with 16 water molecules.

E = -1422.281981
H = -1422.281037

O	1.119784	-0.938000	1.272214
Mg	-0.671580	-0.443768	0.383906
O	-1.896909	-0.710697	2.023296
O	-0.601877	1.584021	0.755908
O	-2.465416	-0.057700	-0.827641
O	0.348935	-0.328212	-1.470307
O	-0.890910	-2.600519	-0.046847
O	1.981894	-0.469513	3.761620
O	1.326712	3.426482	0.396958
O	-3.307446	2.084131	0.567525
O	-3.744900	1.151794	3.023290
O	-6.121570	0.271709	3.795490
O	-1.573748	-0.480352	-3.376820
O	1.768090	-3.210718	-0.166318
O	2.932812	-1.511664	-2.006817
O	-2.809954	-2.495366	-1.999803

H	1.521488	-1.788481	1.029546
H	1.395882	-0.711593	2.188143
H	1.264666	-0.595181	-1.642255
H	-0.149159	-0.351007	-2.309756
H	-2.257791	0.188009	-1.748308
H	-2.948030	0.693989	-0.409610
H	0.133005	2.218394	0.611956
H	-1.446891	2.062261	0.702950
H	-2.498293	-0.069797	2.444076
H	-2.223350	-1.621414	2.216365
H	-1.456334	-2.764724	-0.829373
H	-0.003348	-2.983911	-0.209406
H	-3.603540	1.836826	1.477807
H	-3.844557	2.821721	0.266169
H	-3.435866	1.692833	3.756026
H	-4.630046	0.797871	3.294471
H	2.189801	-4.048605	0.044339
H	2.279670	-2.785420	-0.881719
H	3.711700	-1.043388	-1.687103
H	3.124624	-1.748657	-2.920688
H	-1.695115	-0.171404	-4.278714
H	-2.010589	-1.347186	-3.282113
H	-3.494851	-3.153314	-2.154201
H	-3.189595	-1.777142	-1.463232
H	-6.924797	0.797540	3.825717
H	-6.304160	-0.539316	4.276126
H	2.771073	0.014565	4.015480
H	1.539754	-0.723320	4.574771

H	1.717837	3.933865	1.112213
H	1.510368	3.909543	-0.412100
O	-2.566784	-3.258676	2.080596
H	-2.480908	-3.952178	2.738521
H	-1.924583	-3.429759	1.374165

Mg^{2+} $(H_2O)_{17}$

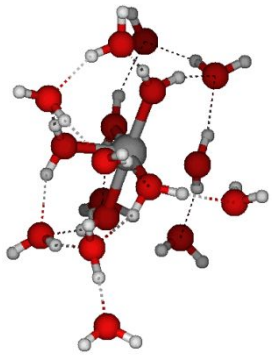


Figure S_{64} : Mg^{2+} optimized structure with 17 water molecules.

E = -1498.701503
H = -1498.700559

O	1.185264	-1.037217	0.983786
Mg	-0.604689	-0.563845	0.133760
O	0.287743	-0.584313	-1.776116
O	-1.730019	-0.728389	1.963750
O	-0.488987	1.482646	0.445867
O	-2.439569	-0.183313	-0.949627
O	-0.859075	-2.731411	-0.164713
O	-2.130772	-3.278745	2.222494
O	2.385812	0.388432	2.801273
O	-3.145263	2.102518	0.233636
O	-3.628339	1.124720	2.622298

O	-6.014030	0.928289	3.778324
O	0.715353	2.539531	2.661026
O	-1.773891	-0.728875	-3.534707
O	-2.901783	-2.723219	-2.011086
O	1.798372	-3.307302	-0.462203
O	2.886058	-1.623974	-2.386109
H	1.613806	-1.876402	0.753564
H	1.709915	-0.550142	1.674114
H	1.216337	-0.758789	-1.993377
H	-0.240402	-0.581853	-2.595003
H	-2.289217	-0.063835	-1.908687
H	-2.877234	0.636120	-0.613158
H	0.045535	1.943896	1.124598
H	-1.322607	1.975819	0.330456
H	-2.573198	-0.235547	2.068645
H	-1.904717	-1.676933	2.217353
H	-1.480331	-2.925053	-0.896441
H	0.023898	-3.093297	-0.395398
H	-3.462964	1.881314	1.147680
H	-3.649257	2.849009	-0.101260
H	-3.011869	1.422015	3.312240
H	-4.521859	1.024071	3.033668
H	2.232329	-4.146425	-0.282984
H	2.268082	-2.878898	-1.204033
H	3.670124	-1.132942	-2.116962
H	3.040631	-1.882723	-3.301249
H	-1.978681	-0.411183	-4.418688
H	-2.184344	-1.603652	-3.412991

H	-3.559230	-3.416306	-2.129695
H	-3.309649	-2.007998	-1.497842
H	-6.583226	1.671883	3.991619
H	-6.461766	0.139372	4.092949
H	2.014134	1.290332	2.809632
H	3.304174	0.433103	3.074109
H	0.039983	2.207912	3.294750
H	0.872069	3.471610	2.837389
H	-1.950951	-3.939636	2.894902
H	-1.627204	-3.498349	1.422278
H	-1.105675	0.317237	3.428684
O	-1.156390	1.120895	3.984088
H	-1.013124	0.850585	4.896414

Mg^{2+} $(H_2O)_{18}$

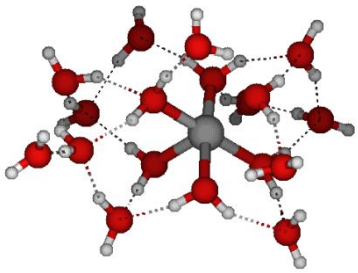


Figure S_{65} : Mg^{2+} optimized structure with 18 water molecules.

E = -1575.114696
H = -1575.113752

O	1.279530	-0.912325	0.881548
Mg	-0.620650	-0.536490	0.095318
O	-2.488199	-0.156996	-0.897406
O	0.186469	-0.584708	-1.836257

O	-1.673419	-0.696637	1.976901
O	-0.460025	1.507371	0.449365
O	-0.868917	-2.708731	-0.123341
O	-2.113483	-3.238284	2.272079
O	1.999004	0.111805	3.155502
O	-3.102893	2.175456	0.255607
O	-3.635986	1.114625	2.598843
O	-6.074985	0.836314	3.620956
O	-1.973677	-0.745229	-3.495518
O	0.679760	2.457963	2.777050
O	-1.251953	1.125688	4.076441
O	1.748989	-3.272395	-0.392470
O	-2.963660	-2.783120	-1.925965
O	2.661092	-1.648892	-2.284031
H	1.619902	-1.807860	0.680820
H	1.571549	-0.630381	1.793961
H	1.069134	-0.906403	-2.113409
H	-0.398102	-0.578117	-2.614974
H	-2.403816	-0.091532	-1.870404
H	-2.897335	0.682402	-0.578776
H	0.034921	1.918977	1.186241
H	-1.287921	2.010743	0.327871
H	-2.520832	-0.205956	2.062250
H	-1.857624	-1.641835	2.235263
H	-1.497136	-2.913481	-0.845858
H	0.010682	-3.093175	-0.344228
H	-3.435512	1.937034	1.159377
H	-3.598220	2.930331	-0.073459

H	-3.063955	1.405377	3.328640
H	-4.546339	0.979586	2.960352
H	2.224392	-4.078814	-0.173466
H	2.183397	-2.860420	-1.179509
H	3.195001	-0.982933	-1.770303
H	3.104348	-1.826752	-3.118379
H	-2.195772	-0.440097	-4.379786
H	-2.340383	-1.637529	-3.368807
H	-3.565416	-3.525154	-2.046049
H	-3.430140	-2.107910	-1.412702
H	-6.672453	1.564675	3.808099
H	-6.509817	0.037618	3.928969
H	1.778719	1.062460	3.119570
H	2.830134	0.003909	3.623574
H	-0.046120	2.192932	3.386467
H	0.906247	3.376454	2.950433
H	-1.950537	-3.906900	2.941131
H	-1.632267	-3.474776	1.463042
H	-1.144184	0.320954	3.532544
H	-1.129160	0.871827	4.996485
H	2.817698	0.105931	0.008104
O	3.586126	0.066714	-0.579640
H	3.924638	0.956688	-0.701832

Mg^{2+} $(H_2O)_{19}$

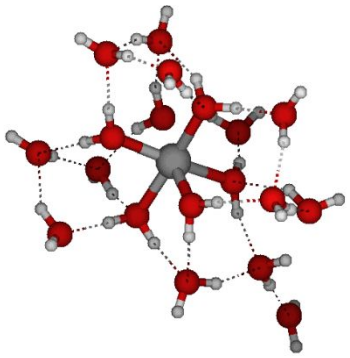


Figure S_{66} : Mg^{2+} optimized structure with 19 water molecules.

E = -1651.526333
H = -1651.525389

O	1.264669	-0.944361	1.029714
Mg	-0.551825	-0.343551	0.172611
O	-0.284464	1.634152	0.778906
O	-2.289943	0.350170	-0.864338
O	0.389393	-0.370578	-1.711823
O	-1.676102	-0.646114	2.006436
O	-0.974922	-2.465776	-0.236709
O	1.891976	-0.257957	3.464065
O	-2.265895	-3.177487	2.080380
O	-2.931020	2.385100	0.765250
O	-3.570414	1.085735	2.948621
O	-6.034421	0.748731	3.881607
O	1.621308	-3.210469	-0.428270
O	2.885979	-1.489022	-2.004864
O	3.798116	-0.051510	-0.051227
O	-1.151570	-0.952829	-3.950331
O	0.823885	2.227493	3.246524

O	-1.176105	0.833434	4.368054
O	-2.886587	-1.984171	-2.117613
H	1.530874	-1.847091	0.757054
H	1.491745	-0.799867	1.989842
H	1.312992	-0.651987	-1.871316
H	-0.086479	-0.524555	-2.551291
H	-2.116453	0.853303	-1.717950
H	-2.766898	1.007657	-0.306534
H	0.213906	1.916983	1.571559
H	-1.113169	2.151861	0.756156
H	-2.495343	-0.133844	2.188748
H	-1.902490	-1.602564	2.169307
H	-1.607521	-2.538346	-0.982750
H	-0.123858	-2.890505	-0.484617
H	-3.291776	2.061434	1.630075
H	-3.405427	3.180718	0.509350
H	-2.999908	1.251172	3.717112
H	-4.491893	0.933385	3.273533
H	2.009244	-4.071367	-0.247553
H	2.171960	-2.763046	-1.116484
H	3.425363	-0.937059	-1.376231
H	3.387419	-1.609979	-2.815964
H	-0.912218	-1.359006	-4.787922
H	-1.860839	-1.487613	-3.539313
H	-3.735712	-2.422883	-2.227860
H	-3.034034	-1.133652	-1.652222
H	-6.613631	1.461072	4.163554
H	-6.511323	-0.070796	4.032410

H	1.779335	0.711358	3.503521
H	2.687393	-0.495707	3.946459
H	0.064886	1.941457	3.803713
H	1.100549	3.103386	3.531618
H	-2.161821	-3.924124	2.674099
H	-1.813942	-3.369872	1.243938
H	-1.092270	0.112666	3.714618
H	-1.030084	0.449163	5.238149
H	2.979745	0.004629	0.462761
H	4.228489	0.806485	-0.041032
H	-1.620606	2.325386	-3.421986
O	-2.031402	1.494482	-3.173404
H	-1.716022	0.802422	-3.781160

Ca^{2+} (H_2O)

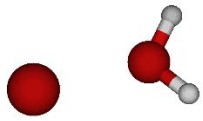


Figure S_{67} : Ca^{2+} optimized structure with 1 water molecule.

E = -112.612598
H = -112.611654

Ca	-0.110102	0.000000	-0.168444
O	0.099127	0.000000	2.038626
H	0.922431	0.000000	2.563995
H	-0.612895	0.000000	2.707177

Ca^{2+} $(H_2O)_2$

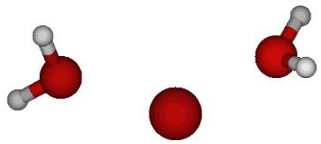


Figure S_{68} : Ca^{2+} optimized structure with 2 water molecules.

E = -189.066054
H = -189.065109

O	0.071916	-0.118496	2.257343
Ca	0.010969	0.065782	0.007284
H	0.827750	-0.374374	2.815807
H	-0.656649	0.025148	2.887664
O	0.793309	1.750540	-1.270898

H	0.847341	1.789615	-2.242717
H	1.150882	2.606493	-0.974372

Ca^{2+} $(H_2O)_3$

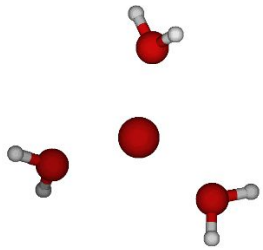


Figure S_{69} : Ca^{2+} optimized structure with 3 water molecules.

E = -265.509450
H = -265.508506

O	0.070970	-0.091605	2.231442
Ca	-0.065735	-0.067463	-0.052560
O	0.854995	1.669168	-1.223354
H	0.815782	0.195859	2.785631
H	-0.602565	-0.392252	2.864267
H	1.324292	1.630874	-2.073551
H	0.863334	2.610569	-0.982101
O	-1.114714	-1.786464	-1.138263
H	-1.695437	-1.733192	-1.915760
H	-1.078841	-2.733943	-0.924871

Ca^{2+} $(H_2O)_4$

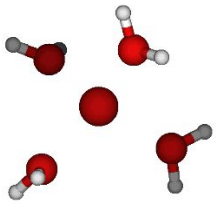


Figure S_{70} : Ca^{2+} optimized structure with 4 water molecules.

E = -341.942811
H = -341.941867

O	0.668360	-0.585933	2.217080
Ca	-0.345441	0.244725	0.309396
O	-1.132530	-1.588136	-0.865283
O	1.154558	1.466606	-0.961431
H	1.526879	-0.329069	2.588486
H	0.337098	-1.276574	2.812155
H	1.584911	1.196629	-1.787804
H	1.479426	2.365165	-0.794472
H	-2.004867	-1.695674	-1.275713
H	-0.670099	-2.422063	-1.042904
O	-2.075513	1.684709	0.850837
H	-2.530549	2.311507	0.266982
H	-2.494400	1.803904	1.717612

Ca^{2+} $(H_2O)_5$

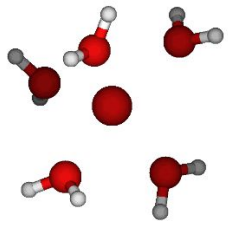


Figure S_{71} : Ca^{2+} optimized structure with 5 water molecules.

E = -418.361494
H = -418.360550

O	1.069265	-1.141286	1.772823
Ca	-0.429588	0.391904	0.759809

O	1.082261	1.510222	-0.632798
O	-1.250927	-1.399195	-0.505573
O	-2.408820	1.569320	0.196021
H	2.018644	-1.213419	1.597477
H	0.883720	-1.819676	2.438168
H	1.324930	1.281552	-1.542160
H	1.599756	2.301693	-0.423310
H	-2.023809	-1.400586	-1.088002
H	-0.888827	-2.295117	-0.558217
H	-2.481351	2.297160	-0.438245
H	-3.306874	1.438915	0.533443
O	-0.418629	1.580721	2.777414
H	0.155972	1.433855	3.542159
H	-0.987933	2.323586	3.023592

Ca^{2+} $(H_2O)_6$

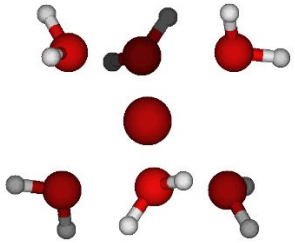


Figure S_{72} : Ca^{2+} optimized structure with 6 water molecules.

E = -494.774601
H = -494.773657

O	1.402221	-0.974673	1.916354
Ca	-0.160194	0.213458	0.560362
O	1.424673	1.971645	0.269438
O	-1.747696	-1.542671	0.851039

O	-1.006707	1.309247	2.502370
O	-1.722141	1.401326	-0.796102
H	2.298115	-0.701232	2.155200
H	1.270968	-1.831727	2.343772
H	2.091489	2.051149	-0.425909
H	1.536907	2.754100	0.825848
H	-2.412965	-1.622357	1.547858
H	-1.862111	-2.324324	0.293946
H	-1.590344	2.257643	-1.224824
H	-2.618524	1.128468	-1.033780
H	-0.708416	1.194912	3.414726
H	-1.720755	1.959579	2.543573
O	0.688521	-0.883766	-1.379606
H	0.391661	-0.769984	-2.292502
H	1.401845	-1.534990	-1.419200

Ca^{2+} $(H_2O)_7$

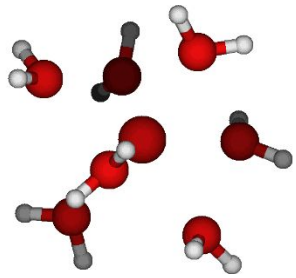


Figure S_{73} : Ca^{2+} optimized structure with 7 water molecules.

E = -571.161906
H = -571.166962

O	1.567735	-0.782605	2.129744
Ca	-0.147251	-0.157993	0.567728
O	1.087722	1.902202	0.324773

O	1.304564	-0.493650	-1.436651
O	-2.163819	-1.082350	1.521855
O	-0.925316	1.294420	2.453566
O	-1.649161	0.785743	-1.054255
H	2.304263	-0.251560	2.457855
H	1.718171	-1.675068	2.466848
H	1.734304	2.107524	-0.361320
H	1.041295	2.681544	0.891666
H	-2.542435	-0.626650	2.283695
H	-2.755057	-1.819220	1.326267
H	-1.562295	1.621207	-1.530319
H	-2.532363	0.456185	-1.264349
H	-0.581686	1.267617	3.355845
H	-1.541791	2.037659	2.432992
H	1.023324	-0.376034	-2.353091
H	2.246654	-0.702066	-1.478832
O	-0.106115	-2.508710	0.014243
H	0.393508	-2.789986	-0.761969
H	-0.482244	-3.310307	0.397386

Ca^{2+} $(H_2O)_8$

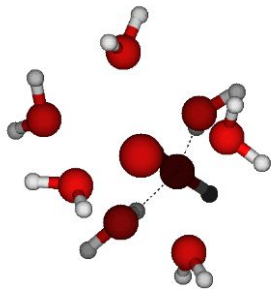


Figure S_{74} : Ca^{2+} optimized structure with 8 water molecules.

E = -647.570531

H = -647.569857

O	1.014267	0.143531	2.009778
Ca	-0.274475	0.236860	0.018054
O	-1.384732	0.095041	-2.110468
O	1.184312	2.054845	-0.610490
O	-1.975597	-0.094830	1.799248
O	-0.727182	-2.136869	-0.195152
O	1.616088	-0.892912	-1.180015
O	-0.591527	-0.487191	4.162292
H	1.855435	0.576757	2.193052
H	0.628963	-0.110015	2.874970
H	1.960627	2.050925	-1.182548
H	1.085490	2.962620	-0.298999
H	-1.665721	-0.275231	2.712577
H	-2.880197	-0.424794	1.744367
H	-1.673671	0.787303	-2.717683
H	-1.786940	-0.723043	-2.427668
H	-0.536163	-1.349171	4.597199
H	-0.690577	0.155650	4.878204
H	1.728729	-0.941019	-2.137798
H	2.461547	-1.168581	-0.803849
H	-0.006819	-2.661564	-0.565815
H	-1.327574	-2.757913	0.233014
O	-1.556282	2.250436	0.402774
H	-1.844308	3.062347	-0.030337
H	-2.159410	2.096372	1.141671

Ca^{2+} $(H_2O)_9$

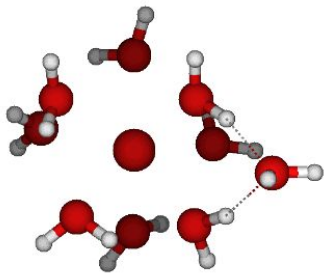


Figure S_{75} : Ca^{2+} optimized structure with 9 water molecules.

E = -723.960264
H = -723.959320

O	1.022596	-0.098044	1.844940
Ca	-0.560186	-0.031821	0.038309
O	-0.522187	0.510575	-2.420405
O	0.812990	2.012053	-0.561191
O	-1.727266	2.155682	0.423427
O	-0.782748	-2.518293	0.142528
O	-1.856875	0.082794	2.178223
O	1.194866	-1.253482	-1.289670
O	-0.173431	-0.127122	4.347140
H	1.982314	-0.023871	1.814422
H	0.774643	-0.143473	2.791171
H	1.740402	2.275990	-0.532067
H	0.310535	2.716861	-0.127284
H	-1.442678	-0.002315	3.063274
H	-2.724019	-0.337019	2.228269
H	-0.069123	1.365256	-2.466751
H	-1.142329	0.472823	-3.158393
H	-0.143340	-0.906849	4.917990
H	-0.064060	0.629677	4.939094
H	1.020404	-0.930877	-2.186904

H	2.121318	-1.520743	-1.259677
H	-0.058274	-2.813232	-0.428252
H	-0.879080	-3.184375	0.833341
H	-2.356325	2.740465	-0.015960
H	-2.095081	1.950460	1.297533
O	-2.766205	-0.825978	-0.622519
H	-2.741812	-1.790278	-0.686518
H	-3.559927	-0.529086	-1.08166

Ca^{2+} $(H_2O)_{10}$

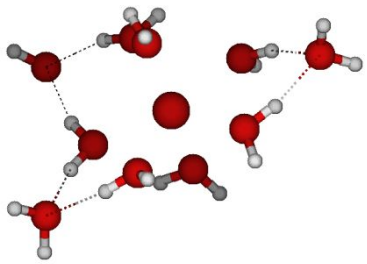


Figure S_{76} : Ca^{2+} optimized structure with 10 water molecules.

E = -800.370142
H = -800.369198

O	1.231045	-0.159156	1.829531
Ca	-0.352422	-0.076059	0.027586
O	-4.290729	0.042772	1.810345
O	-0.760213	-2.435328	-0.123218
O	-1.628746	-0.877982	1.981894
O	-2.598340	0.847909	-0.220127
O	1.763197	-0.103401	-1.121679
O	1.343282	0.587512	-3.780346
O	-0.248310	2.315856	0.098042
O	0.069293	-0.904618	4.220482

H	2.123267	0.200530	1.864447
H	0.984452	-0.398291	2.746471
H	0.389277	3.017720	0.267704
H	-1.122424	2.722047	0.045912
H	-1.223555	-0.926278	2.868431
H	-2.566293	-0.632628	2.099134
H	1.488056	1.496830	-4.073861
H	1.658341	0.030698	-4.504812
H	0.317633	-1.740541	4.636954
H	-0.002933	-0.267224	4.942980
H	1.817538	0.143601	-2.066971
H	2.593381	-0.535208	-0.895130
H	-0.400002	-3.245708	-0.499591
H	-1.220083	-2.668552	0.694998
H	-2.930508	0.895197	-1.123984
H	-3.355781	0.664871	0.371101
H	-5.003206	-0.592938	1.662055
H	-4.659834	0.706858	2.407324
O	-0.955443	-0.093894	-2.358288
H	-1.410818	-0.849488	-2.746903
H	-0.286661	0.186151	-3.015349

$Ca(H_2O)_{11}$

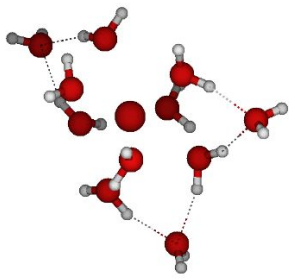


Figure S_{77} : Ca^{2+} optimized structure with 11 water molecules.

E = -876.752275
H = -816.751331

O	1.197283	-0.140257	2.026511
Ca	-0.425822	0.391289	0.335971
O	0.611076	2.476420	-0.298063
O	-0.648070	-2.015994	-0.338587
O	1.732471	0.201683	-1.097691
O	-2.815768	0.921754	0.052614
O	-1.187517	0.174144	-2.032023
O	-1.683040	-1.210899	1.930016
O	-0.019728	-1.397214	4.177998
O	-4.433504	-0.678820	1.654191
O	1.007716	0.335538	-3.798555
H	2.063684	0.246873	2.189526
H	0.908539	-0.552440	2.866933
H	1.436557	2.253885	-0.749773
H	0.503456	3.432880	-0.311316
H	-1.300502	-1.346937	2.817759
H	-2.648248	-1.097767	2.028279
H	1.227216	1.141536	-4.284284
H	1.129385	-0.381778	-4.434520
H	0.298598	-2.263245	4.465510
H	-0.194149	-0.903577	4.989971
H	1.624896	0.161183	-2.070241
H	2.538681	-0.283446	-0.889886
H	-0.038023	-2.735636	-0.533067
H	-1.107090	-2.237199	0.494387
H	-2.998894	0.983630	-0.894138

H	-3.549627	0.430197	0.471018
H	-4.981972	-1.389905	1.297459
H	-4.983232	-0.242136	2.318005
H	-1.336066	-0.782482	-2.032467
H	-0.607877	0.344949	-2.797546
O	-1.261536	1.991004	2.002782
H	-2.099055	2.316502	1.647070
H	-0.851210	2.721424	2.477958

Ca^{2+} $(H_2O)_{12}$

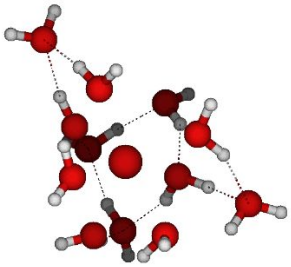


Figure S_{78} : Ca^{2+} optimized structure with 12 water molecules.

E = -953.151672
H = -953.150728

O	1.559935	-0.102841	1.874752
Ca	-0.161185	0.791625	0.495404
O	0.322611	3.079655	-0.059059
O	-0.653806	1.779161	2.808106
O	-2.479341	1.633838	0.801425
O	-0.979569	0.023817	-1.553248
O	-1.287247	-3.281598	-0.367384
O	-1.276624	-1.151679	1.525033
O	1.788825	1.001662	-1.038154
O	-0.083163	-0.717227	3.934834

O	-3.842656	-0.648033	0.852028
O	1.076802	-0.011256	-3.482603
H	2.421535	-0.511965	1.745903
H	1.222107	-0.407547	2.744705
H	1.064913	3.027807	-0.677263
H	0.068112	4.006024	0.011492
H	-0.993070	-1.238820	2.460343
H	-2.259868	-1.100989	1.506823
H	1.039220	0.563144	-4.258853
H	1.439179	-0.850234	-3.796322
H	-0.002747	-1.127916	4.804582
H	-0.402233	0.192870	4.056324
H	1.695778	0.662169	-1.955893
H	2.726710	0.955301	-0.820883
H	-1.351435	-4.214446	-0.134125
H	-1.125492	-2.783771	0.453308
H	-2.842628	2.322718	0.232299
H	-3.150047	0.904232	0.820067
H	-3.787171	-1.076944	-0.042210
H	-4.705735	-0.845457	1.234764
H	-1.771845	-0.551496	-1.657968
H	-0.432809	-0.078396	-2.352632
H	-1.551780	2.054259	2.552034
H	-0.208220	2.563419	3.153062
O	-3.066810	-1.723714	-1.434821
H	-3.597747	-2.033878	-2.178164
H	-2.488896	-2.479677	-1.121276

Ca^{2+} $(H_2O)_{13}$

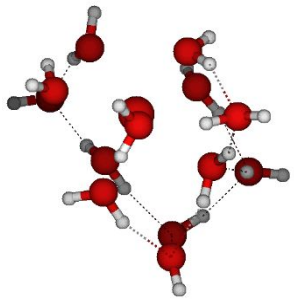


Figure S_{79} : Ca^{2+} optimized structure with 13 water molecules.

E = -1029.541242
H = -1029.540298

O	1.615711	-0.021352	2.107070
Ca	-0.009562	0.504883	0.436544
O	-1.062718	0.162647	-1.687907
O	0.412064	2.853108	-0.025447
O	-1.389368	-1.201487	1.687468
O	-2.312225	1.555491	0.671578
O	1.909849	1.075673	-1.282975
O	-0.674117	1.781263	2.754331
O	-3.865044	-0.622916	0.765226
O	-2.912062	-1.898419	-1.422886
O	-1.136264	-3.327168	0.056967
O	-0.288286	-0.543227	4.043207
O	0.780793	0.768302	-3.782393
H	2.118951	-0.807934	1.862664
H	1.214632	-0.220344	2.976548
H	1.185809	2.747391	-0.603285
H	0.423414	3.750174	0.323292
H	-1.116852	-1.154615	2.636004

H	-2.358154	-1.042244	1.629950
H	0.586580	1.581959	-4.266617
H	1.099951	0.146841	-4.449818
H	-0.328912	-0.828646	4.963841
H	-0.576952	0.388838	3.990965
H	1.697579	0.976042	-2.235685
H	2.868612	1.023975	-1.193189
H	-1.148771	-4.260743	0.302161
H	-1.280760	-2.792716	0.870698
H	-2.494593	2.198147	-0.024208
H	-3.056038	0.907796	0.666564
H	-3.759169	-1.119139	-0.080766
H	-4.771849	-0.735638	1.074083
H	-1.743675	-0.533856	-1.789913
H	-0.596605	0.259954	-2.536188
H	-1.508396	2.022967	2.309194
H	-0.264203	2.599055	3.059873
H	-3.430156	-2.308353	-2.126482
H	-2.347360	-2.600754	-1.022318
O	1.025324	-1.672421	-0.147946
H	0.403177	-2.430674	-0.175391
H	1.626415	-1.786276	-0.890801

Ca^{2+} $(H_2O)_{14}$

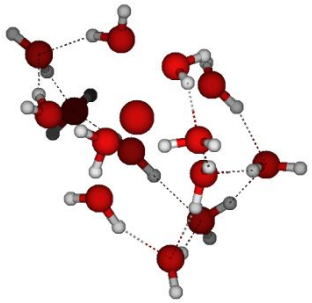


Figure S_{80} : Ca^{2+} optimized structure with 14 water molecules.

E = -1105.937346
H = -1105.936401

O	1.371361	-0.208504	2.693035
Ca	0.078279	0.403796	0.763622
O	-0.660189	-0.027674	-1.487216
O	0.196350	2.740320	-0.071679
O	1.067967	-1.848677	0.465756
O	-1.565367	-1.228595	1.865810
O	-2.220646	1.498524	0.718604
O	2.052202	2.488791	-2.056563
O	-0.814946	1.888227	2.916516
O	-3.848827	-0.615397	0.524053
O	-0.837010	-0.429434	4.326936
O	-1.146960	-3.439671	0.384657
O	-2.585093	-2.032866	-1.410947
O	0.645124	0.972046	-3.883067
H	1.705217	-1.085648	2.458433
H	0.849985	-0.328958	3.509965
H	0.814325	2.832502	-0.830885
H	0.336573	3.522621	0.472768
H	-1.452184	-1.123534	2.840659
H	-2.502621	-1.037976	1.640868

H	0.066394	1.449203	-4.492781
H	1.156004	0.367352	-4.437663
H	-1.057789	-0.621668	5.245852
H	-1.002124	0.519529	4.157137
H	1.652406	2.043524	-2.834064
H	2.663537	3.158505	-2.385877
H	-1.247426	-4.355437	0.671929
H	-1.371108	-2.851123	1.142074
H	-2.165503	2.128779	-0.010229
H	-2.987854	0.902951	0.557727
H	-3.610354	-1.150409	-0.269104
H	-4.794533	-0.714789	0.684106
H	-1.323676	-0.730501	-1.647135
H	-0.263161	0.211914	-2.342076
H	-1.602279	2.055111	2.361009
H	-0.553604	2.725149	3.318168
H	-2.995220	-2.474936	-2.164175
H	-2.120553	-2.725221	-0.880071
H	0.476148	-2.612850	0.313472
H	1.762634	-1.873370	-0.201499
O	2.358612	0.626752	-0.075155
H	2.504525	1.276547	-0.793647
H	3.092744	0.717760	0.543250

Ca^{2+} $(H_2O)_{15}$

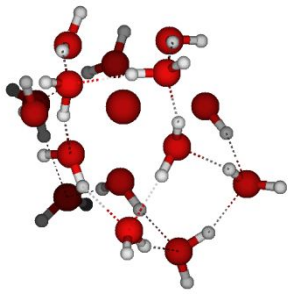


Figure S_{81} : Ca^{2+} optimized structure with 15 water molecules.

E = -1182.334527
H = -1182.333583

O	1.464020	-0.427377	2.688504
Ca	0.392227	0.314988	0.626319
O	-0.587987	-0.165060	-1.512368
O	2.546905	0.594930	-0.432283
O	1.240619	-1.983810	0.330884
O	0.265845	2.623912	-0.418986
O	-1.823145	1.606915	0.939047
O	-1.381943	-1.201066	1.785012
O	-1.409341	2.254093	3.542181
O	-3.602347	-0.386283	0.454473
O	-0.800421	-0.303729	4.265483
O	-1.083402	-3.447438	0.376080
O	-2.571294	-2.072326	-1.403795
O	2.086812	2.383515	-2.450775
O	0.356780	0.938900	-4.044970
H	1.783644	-1.328225	2.551852
H	0.865354	-0.449972	3.461899
H	0.829559	2.788124	-1.201795
H	0.692582	3.066771	0.332391
H	-1.299341	-1.035302	2.753834

H	-2.290551	-0.934086	1.519137
H	-0.271948	1.473129	-4.548342
H	0.717797	0.305118	-4.678853
H	-0.999333	-0.634444	5.149303
H	-1.092441	0.635404	4.222946
H	1.600865	1.935325	-3.174279
H	2.673768	3.035760	-2.851278
H	-1.199202	-4.349805	0.697670
H	-1.271034	-2.825621	1.118923
H	-1.577745	2.251537	0.253230
H	-2.592248	1.086979	0.619115
H	-3.438339	-0.977597	-0.316810
H	-4.544673	-0.418986	0.656008
H	-1.270840	-0.851941	-1.658425
H	-0.332431	0.186460	-2.382272
H	-1.828761	2.156484	2.658121
H	-1.865006	2.960016	4.016444
H	-3.022776	-2.522081	-2.127765
H	-2.114656	-2.761027	-0.862109
H	0.567701	-2.689236	0.234880
H	1.876732	-2.104966	-0.382403
H	2.590597	1.228614	-1.181333
H	3.435815	0.515152	-0.070558
O	0.923243	2.292227	2.160691
H	1.723823	2.136501	2.676021
H	0.209240	2.479770	2.808074

Ca^{2+} $(H_2O)_{16}$

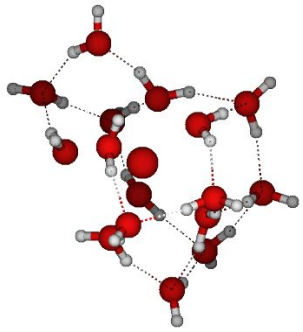


Figure S_{82} : Ca^{2+} optimized structure with 16 water molecules.

E = -1258.726702
H = -1258.725758

O	1.286022	-0.721450	2.039247
Ca	-0.004221	0.581607	0.487895
O	-1.241301	0.094363	-1.462662
O	3.547195	1.442809	-0.943170
O	1.567435	-2.847616	0.308250
O	0.356008	2.706193	-0.514741
O	0.813539	2.175979	2.168371
O	-2.129359	1.826570	1.063173
O	-1.575109	-1.081093	1.622530
O	-1.205229	-3.315430	0.178020
O	-3.081311	-1.918444	-1.313110
O	-0.694028	-0.528577	4.076132
O	-1.390562	2.122364	3.738755
O	-3.920709	-0.219932	0.654389
O	1.860893	2.682689	-2.756775
O	0.765210	0.277846	-3.348274
H	1.527260	-1.609173	1.710891
H	0.891062	-0.814232	2.923093
H	0.819332	2.859255	-1.371741

H	0.815576	3.237109	0.149099
H	-1.378025	-1.022262	2.590803
H	-2.523272	-0.849393	1.490195
H	0.885329	-0.226467	-4.161475
H	1.252951	-0.180972	-2.624372
H	-0.835569	-0.966390	4.923738
H	-0.962801	0.410031	4.181613
H	1.474322	1.902920	-3.217498
H	1.959459	3.390634	-3.404220
H	-1.484033	-4.161849	0.550457
H	-1.353018	-2.627985	0.873906
H	-2.121184	2.584897	0.462391
H	-2.896512	1.267544	0.804180
H	-3.852159	-0.798597	-0.138901
H	-4.834842	-0.252045	0.960481
H	-1.926872	-0.590771	-1.597282
H	-0.745191	0.188191	-2.300785
H	-1.924081	2.168541	2.919561
H	-1.747539	2.768077	4.360885
H	-3.565573	-2.333586	-2.036700
H	-2.489244	-2.597353	-0.917627
H	0.659510	-3.181251	0.143425
H	2.162838	-3.605528	0.273576
H	3.207684	2.015492	-1.659602
H	4.504787	1.398645	-1.036955
H	1.666328	1.985534	2.577035
H	0.182597	2.360712	2.895753
O	1.733284	-0.400390	-0.934904
H	2.571728	0.148422	-0.890155

H	1.908744	-1.316175	-0.629921

Ca^{2+} $(H_2O)_{17}$

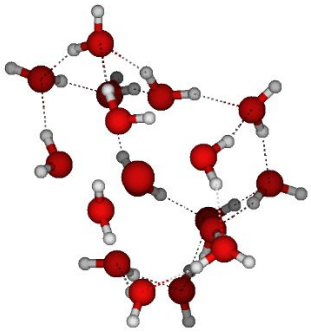


Figure S_{83} : Ca^{2+} optimized structure with 17 water molecules.

E = -1335.116543
H = -1335.115599

O	1.314255	-0.843757	2.089015
Ca	0.166273	0.745490	0.556512
O	-1.212467	0.256356	-1.338880
O	0.431750	2.786744	-0.660103
O	1.670795	-0.582707	-1.074002
O	0.423600	2.423700	2.258780
O	-2.170694	1.773437	1.216553
O	-1.523275	-1.112615	1.581618
O	3.813117	1.068646	-1.297646
O	-0.668595	-0.711797	4.079532
O	-3.913144	-0.262215	0.665844
O	-1.315703	-3.328899	0.140605
O	0.664673	0.309246	-3.398196
O	2.085204	2.516431	-2.827863
O	-1.612784	1.844529	3.934340
O	-3.041652	-1.816159	-1.373887

O	1.396081	-2.938480	0.269788
H	1.402564	-1.732763	1.690942
H	0.864032	-0.933834	2.949571
H	0.979430	2.863559	-1.472527
H	0.706351	3.500116	-0.072121
H	-1.339630	-1.107620	2.552647
H	-2.465534	-0.857707	1.457101
H	0.651917	-0.178053	-4.230149
H	1.100490	-0.252656	-2.715567
H	-0.797926	-1.198928	4.901534
H	-0.995033	0.206246	4.226831
H	1.579277	1.792266	-3.269797
H	2.253443	3.202084	-3.485461
H	-1.654358	-4.145642	0.528729
H	-1.415009	-2.610621	0.822173
H	-2.225877	2.612249	0.740804
H	-2.899646	1.211257	0.872868
H	-3.842372	-0.798995	-0.156063
H	-4.822305	-0.322926	0.980800
H	-1.877999	-0.446726	-1.474020
H	-0.779555	0.394906	-2.202134
H	-2.073516	1.904558	3.070558
H	-2.111706	2.363811	4.575906
H	-3.496460	-2.169566	-2.147227
H	-2.496511	-2.537380	-0.985188
H	0.474700	-3.251524	0.116244
H	1.971980	-3.711624	0.240244
H	3.389459	1.698068	-1.925244
H	4.740765	0.984169	-1.545694

H	1.369684	2.488812	2.447418
H	-0.084091	2.457855	3.090362
H	2.580418	-0.208464	-1.109751
H	1.718740	-1.507303	-0.741156
O	2.572800	1.365386	1.119709
H	2.765640	0.562491	1.626005
H	3.224276	1.408287	0.391549

Ca^{2+} $(H_2O)_{18}$

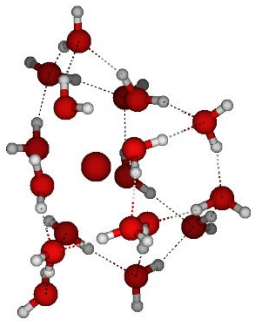


Figure S_{84} : Ca^{2+} optimized structure with 18 water molecules.

E = -1411.510572
H = -1411.509582

O	1.287164	-0.827210	1.972593
Ca	0.160483	0.709940	0.352569
O	0.415333	2.760485	-0.916009
O	-0.985946	0.035297	-1.669061
O	0.262947	2.284867	2.147516
O	2.511338	1.416052	1.043894
O	1.860174	-0.647389	-1.123259
O	-3.261313	2.426495	2.821422
O	1.052689	0.085558	-3.555156
O	2.249270	2.400561	-2.923196

O	-1.242500	1.837040	4.344609
O	-1.552696	-0.923262	1.354536
O	-1.260766	-3.284265	0.135954
O	-0.741532	-0.735310	3.883033
O	-3.822550	-0.206258	0.101549
O	-2.861708	-1.998816	-1.679111
O	3.958688	1.080078	-1.241395
O	1.467139	-2.976561	0.251723
H	1.430451	-1.724110	1.610579
H	0.784685	-0.910868	2.807355
H	1.026356	2.781066	-1.687461
H	0.676361	3.494366	-0.346703
H	-1.433206	-0.906947	2.338738
H	-2.476165	-0.657100	1.135826
H	1.156475	-0.433626	-4.360959
H	1.455128	-0.414574	-2.804951
H	-0.945798	-1.326630	4.616459
H	-0.924931	0.190988	4.194586
H	1.832099	1.629512	-3.380311
H	2.443677	3.066781	-3.593603
H	-1.626184	-4.047374	0.601186
H	-1.398642	-2.489390	0.718185
H	-3.799259	3.215400	2.948429
H	-2.875822	2.480435	1.923984
H	-3.735377	-0.866239	-0.621899
H	-4.747194	-0.174206	0.371932
H	-1.660142	-0.658616	-1.809012
H	-0.475681	0.100589	-2.498170
H	-2.095344	2.104535	3.886280

H	-1.205128	2.285926	5.197025
H	-3.257386	-2.439426	-2.439890
H	-2.354764	-2.668160	-1.166873
H	0.534046	-3.259401	0.112758
H	2.011920	-3.772099	0.268463
H	3.546386	1.668182	-1.913525
H	4.905800	1.047886	-1.417524
H	1.213821	2.408147	2.278510
H	-0.175757	2.274541	3.026357
H	2.764207	-0.264448	-1.085112
H	1.880000	-1.561634	-0.761713
H	2.658225	0.612409	1.567107
H	3.222758	1.455115	0.373598
O	-2.119098	1.917254	0.332981
H	-2.806541	1.296043	0.010524
H	-1.927473	2.530000	-0.390297

Ca^{2+} $(H_2O)_{19}$

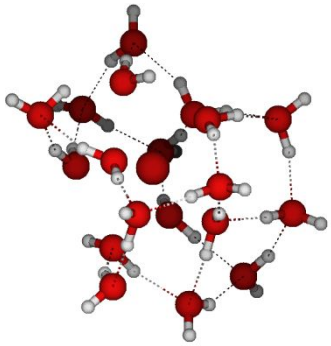


Figure S_{85} : Ca^{2+} optimized structure with 19 water molecules.

E = -1487.902705
H = -1487.901761

O	1.356621	-0.694774	1.949405

Ca	0.098754	0.713729	0.345666
O	0.111274	2.064683	2.296307
O	-1.086057	-0.019070	-1.653292
O	0.244249	2.782125	-0.909309
O	2.517878	1.610998	0.830944
O	-1.522871	-0.990964	1.334028
O	-2.212725	1.863962	0.280211
O	1.778147	-0.679289	-1.152709
O	-0.737346	-0.809418	3.859451
O	-1.607506	1.654144	4.345355
O	-3.545762	2.164303	2.684865
O	0.900454	-0.014327	-3.581030
O	-1.169534	-3.368237	0.185887
O	2.066525	2.332518	-3.009669
O	-3.820907	-0.352858	0.102063
O	-2.833008	-2.175207	-1.638348
O	3.859199	1.034687	-1.437576
O	1.536150	-2.947487	0.321751
H	1.524373	-1.602014	1.628964
H	0.862210	-0.765101	2.788844
H	0.801844	2.771537	-1.713911
H	0.638612	3.461569	-0.320895
H	-1.399089	-0.984305	2.319082
H	-2.452906	-0.741928	1.116343
H	0.989901	-0.550146	-4.377352
H	1.317355	-0.496672	-2.826958
H	-0.880463	-1.448256	4.566870
H	-1.058340	0.069713	4.192239
H	1.642222	1.551685	-3.441564

H	2.234696	2.986678	-3.698607
H	-1.516615	-4.121614	0.679894
H	-1.333880	-2.553162	0.734571
H	-4.151934	2.903893	2.800178
H	-3.091811	2.293656	1.827031
H	-3.749036	-1.039286	-0.596129
H	-4.732458	-0.331176	0.414049
H	-1.710908	-0.762825	-1.762762
H	-0.592323	0.043707	-2.492387
H	-2.439716	1.874444	3.831255
H	-1.645269	2.104820	5.196193
H	-3.204248	-2.636067	-2.399197
H	-2.296047	-2.818003	-1.123736
H	0.614456	-3.274034	0.200443
H	2.116826	-3.717004	0.338919
H	3.396481	1.612612	-2.089979
H	4.794349	1.004943	-1.668360
H	0.484210	2.955669	2.157873
H	-0.443917	2.074044	3.103514
H	2.681864	-0.297435	-1.180924
H	1.827691	-1.577395	-0.751932
H	2.630962	0.955743	1.537147
H	3.195881	1.435768	0.143053
H	-2.846529	1.221620	-0.097969
H	-1.957864	2.476733	-0.425260
O	1.520280	4.072534	1.143306
H	1.924951	4.918067	1.365168
H	2.211001	3.377870	1.152528

Ca^{2+} $(H_2O)_{20}$

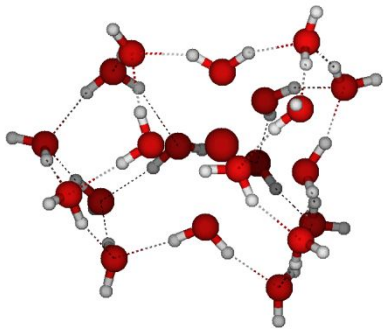


Figure S_{86} : Ca^{2+} optimized structure with 20 water molecules.

E = -1564.292526
H = -1564.291582

O	0.651817	-0.917500	2.567642
Ca	-0.158143	0.426131	0.739742
O	0.071450	2.043812	2.396082
O	0.261899	2.477392	-0.522853
O	-0.774507	-0.406057	-1.426006
O	-2.035576	-1.074046	1.540630
O	-2.291319	1.719914	0.365558
O	3.636551	1.769012	0.667014
O	3.136898	-0.610560	-2.481802
O	-1.620024	-0.734253	4.148841
O	-1.684825	1.891638	4.472597
O	-3.523246	2.522819	2.741014
O	-1.381555	-3.466625	0.550359
O	0.860750	0.101085	-3.663314
O	1.901099	3.614209	1.283804
O	1.518058	2.629047	-3.016518
O	-3.983664	-0.377367	-0.192927

O	3.992869	1.878668	-2.179551
O	-2.698926	-2.365291	-1.564694
O	1.351661	-3.103919	1.099960
H	0.961327	-1.821102	2.375759
H	0.067837	-0.953492	3.347746
H	0.641694	2.572300	-1.419729
H	0.775008	3.098410	0.047324
H	-2.069775	-0.980970	2.528576
H	-2.900345	-0.813103	1.150494
H	0.653433	-0.218964	-4.549088
H	1.718762	-0.310172	-3.389370
H	-1.962705	-1.255130	4.883349
H	-1.687431	0.224489	4.407779
H	1.210528	1.792363	-3.442049
H	1.295345	3.356858	-3.609072
H	-1.780454	-4.222474	0.999307
H	-1.653831	-2.653640	1.054769
H	-4.001383	3.358373	2.728802
H	-3.102746	2.417191	1.864575
H	-3.742105	-1.098653	-0.813796
H	-4.944869	-0.360348	-0.123285
H	-1.435999	-1.098255	-1.627455
H	-0.268413	-0.246298	-2.246341
H	-2.447828	2.224440	3.914267
H	-1.709635	2.346071	5.322039
H	-2.967024	-2.897812	-2.321994
H	-2.276572	-2.966910	-0.907374
H	0.466098	-3.399743	0.800998
H	1.881144	-3.890483	1.270962

H	3.201114	2.342919	-2.538579
H	4.776039	2.290161	-2.563855
H	0.741753	2.751064	2.285053
H	-0.368075	2.116020	3.266164
H	3.634462	0.248312	-2.441023
H	3.767273	-1.301873	-2.715810
H	3.246782	0.882452	0.738477
H	3.894972	1.858681	-0.267246
H	-2.940441	1.174480	-0.121913
H	-1.841453	2.319413	-0.251267
H	2.273392	4.474490	1.503352
H	2.655288	2.972120	1.126215
O	1.997877	-0.582263	0.073466
H	2.352978	-0.663850	-0.836190
H	1.979843	-1.494262	0.430149

$Cl^-(H_2O)$

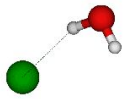


Figure S_{87} : Cl^- optimized structure with 1 water molecule.

E = -91.512984
H = -91.512040

Cl	-0.649291	0.000000	-0.251105
H	0.870475	0.000000	1.437539
O	1.201069	0.000000	2.359619
H	0.369090	0.000000	2.837272

$Cl^-(H_2O)_2$

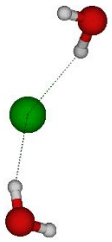


Figure S_{88} : Cl^- optimized structure with 2 water molecules.

E = -167.922326
H = -167.921382

O	1.134140	-0.232321	2.629025
Cl	-0.543779	0.064776	-0.089069
H	0.645299	-0.401915	1.800522
H	1.040523	0.720159	2.696822
H	-2.788489	0.413486	-0.268952
O	-3.734873	0.196878	-0.377483
H	-3.693579	-0.761063	-0.412109

$Cl^-(H_2O)_3$

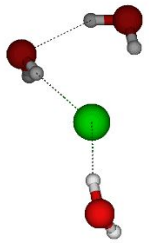


Figure S_{89} : Cl^- optimized structure with 3 water molecules.

E = -244.333935
H = -244.332991

O	1.480863	-0.155569	2.287681
Cl	-1.290082	0.045461	0.286203
O	-4.394216	0.072002	-0.580261
H	0.531347	-0.217095	2.115505
H	1.795546	0.228148	1.455785
H	-3.497752	0.350651	-0.320621
H	-4.293829	-0.882069	-0.584714
H	0.732131	0.648467	-0.393993
O	1.699432	0.571954	-0.539998
H	1.788884	-0.363773	-0.737050

$Cl^-(H_2O)_4$

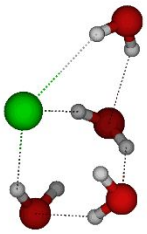


Figure S_{90} : Cl^- optimized structure with 4 water molecules.

E = -320.751327
H = -320.750383

O	1.639905	-0.479970	2.014080
O	0.571905	-0.001875	-0.759808
Cl	-1.393970	1.250096	1.416010
O	-1.926216	-1.350082	-0.587207
H	0.836096	-0.001622	2.253774
H	1.591138	-0.491382	1.049281
H	-1.972803	-0.911607	0.277464
H	-2.169634	-0.623157	-1.188061
H	0.192459	0.582202	-0.074582
H	-0.076932	-0.731137	-0.759551
H	-1.990166	1.529182	-0.926333
O	-1.879807	1.209743	-1.838960
H	-0.933832	0.999069	-1.859409

$Cl^-(H_2O)_5$

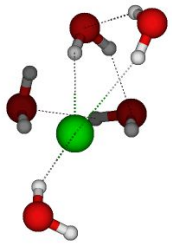


Figure S_{91} : Cl^- optimized structure with 5 water molecules.

E = -397.156483
H = -397.155539

O	1.750113	-0.787471	1.780304
O	0.664576	-0.009019	-0.920125
O	-1.777919	-1.461117	-0.866361

O	-1.838544	1.188771	-1.887568
Cl	-1.326060	0.970243	1.384103
H	0.950609	-0.341007	2.083844
H	1.695839	-0.684157	0.821401
H	-1.862150	-1.132013	0.040908
H	-2.055260	-0.686466	-1.388699
H	0.293041	0.507872	-0.182074
H	0.031921	-0.751262	-0.970952
H	-1.966497	1.452585	-0.961747
H	-0.883795	1.022902	-1.919616
H	-2.089223	2.507079	2.982229
O	-2.599885	2.791839	3.757205
H	-3.005757	1.967087	4.031756

$Cl^-(H_2O)_6$

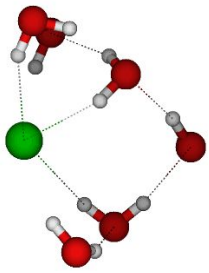


Figure S_{92} : Cl^- optimized structure with 6 water molecules.

E = -473.569217
H = -473.568272

O	-0.809345	0.840891	0.330075
O	0.064513	0.758516	2.937239
O	2.511508	-0.494726	3.431260
O	1.596505	1.249313	5.457232

Cl	2.506460	2.739184	2.674636
O	0.668937	5.460340	1.131151
H	-0.233052	0.177469	-0.055929
H	-0.645613	0.769766	1.296201
H	2.899878	0.261093	2.963060
H	2.374274	-0.124073	4.323152
H	0.603657	1.566314	2.811507
H	0.766122	0.077788	2.999106
H	2.025070	1.945198	4.930379
H	0.747407	1.146933	5.005571
H	0.643756	4.735309	0.483687
H	1.202763	5.081297	1.837158
H	1.621388	2.847707	0.414352
O	0.988393	2.992569	-0.305439
H	0.259589	2.375873	-0.113215

$Cl^-(H_2O)_7$

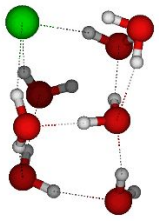


Figure S_{93} : Cl^- optimized structure with 7 water molecules.

E = -549.988961
H = -549.988017

O	-0.388579	0.834386	0.004342
O	0.111526	1.292430	2.644093
O	2.811207	0.547607	3.174965
O	1.001400	0.879883	5.307046

O	1.053548	3.287593	-0.209472
O	0.269984	3.926580	2.341153
Cl	3.124911	3.572009	3.882584
H	0.239518	0.133716	-0.183741
H	-0.365125	0.925595	0.986127
H	3.106719	1.442988	3.449016
H	2.343017	0.250007	3.975051
H	0.076605	2.290661	2.597778
H	1.065440	1.080920	2.622617
H	1.444441	1.734743	5.384262
H	0.395789	1.004840	4.553931
H	0.529893	3.890312	1.391455
H	1.095655	4.088975	2.830686
H	1.937196	2.950261	0.038398
H	0.500365	2.490472	-0.302776
H	3.540585	2.904548	1.634103
O	3.450139	2.307135	0.869937
H	3.305602	1.450076	1.289146

$Cl^-(H_2O)_8$

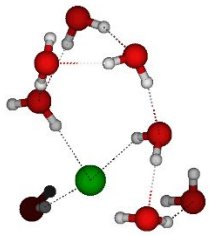


Figure S_{94} : Cl^- optimized structure with 8 water molecules.

E = -626.386999
H = -626.386055

O	-0.300753	-0.111349	0.337968

O	0.247724	0.479200	3.008964
O	-0.105831	-2.920390	-0.003305
O	1.641517	-4.619972	-1.374620
O	2.321975	0.758953	1.103683
O	-0.454604	-5.805991	0.106618
O	2.416830	-1.490791	2.885704
Cl	1.942704	-4.460619	1.995628
H	0.631551	0.156959	0.266413
H	-0.314855	-1.065412	0.140647
H	2.231605	-4.597210	-0.608859
H	0.964921	-5.265648	-1.097047
H	0.381376	-3.146759	0.806330
H	0.496238	-3.254310	-0.698843
H	0.139860	-5.794220	0.871669
H	-0.769539	-4.888660	0.076339
H	1.712682	1.064896	1.798705
H	2.622170	-0.079660	1.487143
H	0.815210	-0.287703	3.178385
H	-0.199517	0.253015	2.167902
H	2.250668	-2.411411	2.591763
H	3.071548	-1.575174	3.581918
O	3.314629	-5.970139	4.541553
H	2.436665	-5.961982	4.928274
H	3.152730	-5.585962	3.666317

$Cl^-(H_2O)_9$

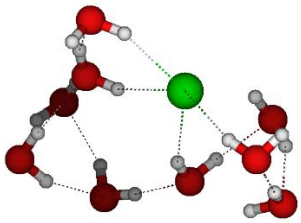


Figure S_{95} : Cl^- optimized structure with 9 water molecules.

E = -702.800899
H = -702.799955

O	-0.157012	-0.183444	0.656678
O	0.433283	0.295893	3.340909
O	2.407748	0.886408	1.382385
O	0.105223	-2.963792	0.116945
O	1.912793	-4.519475	-1.296873
O	-0.584909	-5.655330	-0.864210
O	2.626846	-1.549176	2.833677
Cl	2.042953	-4.741401	2.097628
O	3.653674	-3.517699	4.550907
H	0.750237	0.157089	0.571915
H	-0.117564	-1.123713	0.405101
H	2.341519	-4.718140	-0.453134
H	1.127860	-5.106288	-1.309292
H	0.434755	-3.359736	0.938443
H	0.792707	-3.233125	-0.528522
H	-0.492289	-6.208169	-0.064282
H	-0.763776	-4.762883	-0.530863
H	1.802600	1.098744	2.114070
H	2.803727	0.063743	1.710865
H	1.084407	-0.421118	3.399817

H	-0.032138	0.101601	2.502313
H	2.295708	-2.297275	2.316956
H	3.161522	-1.994278	3.516651
H	2.930269	-3.572642	5.180759
H	3.357339	-4.094029	3.820922
H	0.581132	-6.381848	1.862394
O	0.056137	-7.105005	1.466131
H	0.725891	-7.725624	1.168674

$Cl^-(H_2O)_{10}$

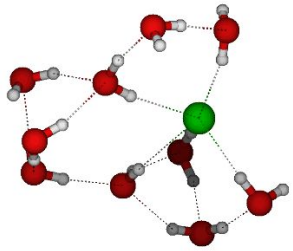


Figure S_{96} : Cl^- optimized structure with 10 water molecules.

E = -779.210060
H = -779.209116

O	0.256947	-0.077160	0.246142
O	0.241826	0.280946	3.029762
O	2.707441	0.453044	1.613305
O	2.194599	-1.867406	3.133037
O	3.219425	-2.990373	5.451540
O	0.160145	-2.881401	-0.260658
O	1.769748	-4.798388	-1.470474
O	-0.920742	-5.424517	-1.187503
O	-0.737125	-6.863557	1.235841
Cl	1.648597	-4.901682	1.932330

H	1.203200	0.076451	0.416843
H	0.183527	-1.011283	-0.016736
H	2.087840	-5.018476	-0.584461
H	0.888859	-5.225850	-1.519162
H	0.389149	-3.245197	0.606962
H	0.843725	-3.280284	-0.838257
H	-0.999450	-5.950046	-0.368833
H	-0.942819	-4.500546	-0.891984
H	2.008121	0.817521	2.181844
H	2.820037	-0.424376	2.018067
H	0.733612	-0.533392	3.223975
H	-0.024398	0.167059	2.095978
H	1.978975	-2.703331	2.691606
H	2.622844	-2.136888	3.971483
H	2.435981	-3.124902	5.989247
H	3.441113	-3.881033	5.098062
H	-0.114292	-6.231338	1.643077
H	-0.176519	-7.608504	1.005642
H	2.971213	-5.377124	3.577611
O	3.674964	-5.405714	4.259604
H	4.487679	-5.374074	3.748969

$Cl^-(H_2O)_{11}$

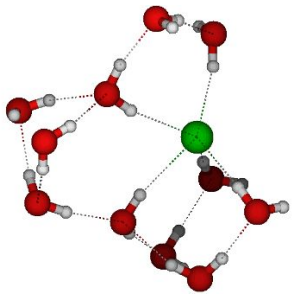


Figure S_{97} : Cl^- optimized structure with 11 water molecules.

E = -855.615745
H = -855.614801

O	0.405792	-0.134309	0.271085
O	-0.063703	0.266800	2.994084
O	2.585530	0.570029	2.000903
O	1.965397	-1.783158	3.448245
O	2.756223	-2.894548	5.863903
O	3.882840	-5.047817	4.607936
O	0.549549	-2.905922	-0.257518
O	1.481623	-4.640102	-2.146712
O	-0.954437	-5.271729	-0.939436
O	-0.672337	-6.551639	1.586178
Cl	1.967859	-4.854220	2.128495
H	1.307048	0.078046	0.568891
H	0.425140	-1.073345	0.011172
H	2.201419	-5.120897	-1.701045
H	0.659039	-5.102601	-1.892827
H	0.956071	-3.314321	0.519707
H	1.019271	-3.317724	-1.019641
H	-0.946242	-5.786343	-0.112778
H	-0.805176	-4.356584	-0.650175
H	1.775412	0.891332	2.432498
H	2.678507	-0.296358	2.431836
H	0.423343	-0.519539	3.286589
H	-0.169999	0.120238	2.032252
H	1.888788	-2.618469	2.965260
H	2.278431	-2.040425	4.339358
H	1.935739	-3.224697	6.236485

H	3.213294	-3.688455	5.508175
H	0.032486	-5.959890	1.908047
H	-0.243450	-7.408175	1.530643
H	3.254030	-5.120462	3.861076
H	4.704759	-4.776132	4.191789
H	3.088622	-5.547783	0.318962
O	3.373508	-5.984755	-0.504887
H	3.107779	-6.898814	-0.383457

$Cl^-(H_2O)_{12}$

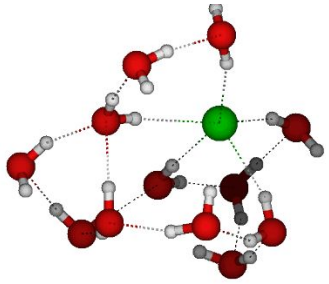


Figure S_{98} : Cl^- optimized structure with 12 water molecules.

E = -932.034709
H = -932.033765

O	-0.057007	-0.816610	0.438194
O	-0.372874	-1.678374	3.016078
O	1.488195	-2.889144	-0.494088
O	1.771334	-4.929202	-2.265365
O	-0.692341	-4.884062	-1.032443
O	2.997705	-6.718191	-0.408675
O	-0.379153	-6.081156	1.435471
O	1.467354	0.760724	2.255600
O	2.458364	-1.640388	3.258718
O	3.456725	-2.597719	5.617391

O	4.501384	-4.886973	4.568460
Cl	2.589507	-4.717335	2.099237
H	0.574541	-0.150008	0.756873
H	0.472701	-1.486720	-0.036101
H	2.294937	-5.574093	-1.757049
H	0.842273	-5.114408	-2.012448
H	1.835898	-3.337463	0.289182
H	1.722913	-3.481744	-1.247226
H	-0.696585	-5.398620	-0.197442
H	-0.367553	-4.014975	-0.760352
H	0.662297	0.619307	2.764893
H	2.036847	0.028530	2.555737
H	0.584030	-1.686537	3.199112
H	-0.425463	-1.457652	2.056457
H	2.630689	-2.416359	2.703287
H	2.848360	-1.867119	4.132642
H	2.699924	-2.888682	6.131224
H	3.896960	-3.425734	5.317991
H	-0.766259	-5.511518	2.133383
H	0.565767	-5.915610	1.559679
H	3.873539	-5.008363	3.826479
H	5.346041	-4.744004	4.134568
H	3.077406	-6.108796	0.345477
H	2.270427	-7.295792	-0.162828
H	-0.735943	-3.388828	3.342998
O	-0.662626	-4.347428	3.560708
H	0.289286	-4.486129	3.616480

$Cl^-(H_2O)_{13}$

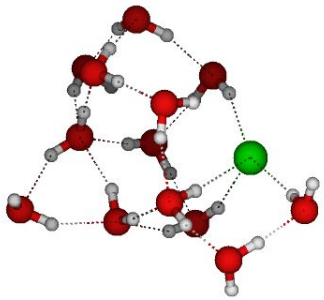


Figure S_{99} : Cl^- optimized structure with 13 water molecules.

E = -1008.453875
H = -1008.452931

O	-0.021522	-2.402198	0.192489
O	0.326201	-2.055904	2.952189
O	-0.306483	-4.765625	3.628858
O	2.280696	-2.358245	-0.931085
O	1.774691	-4.737329	-2.073337
O	-1.027761	-4.224877	-1.834681
O	-0.770652	-5.008516	0.923628
O	2.971684	-2.281470	3.510647
O	4.217038	-2.422382	5.937854
O	4.919306	-5.003759	5.472513
O	-0.636981	0.057082	1.450826
O	1.545851	-6.327908	0.160783
Cl	2.953407	-5.376684	3.076458
H	-0.384664	-1.507624	0.323246
H	0.900611	-2.320905	-0.232561
H	1.837792	-5.368276	-1.322582
H	0.814047	-4.639463	-2.208579
H	3.016081	-2.476725	-0.294846
H	2.217176	-3.206698	-1.441875

H	-1.256740	-4.860077	-1.143243
H	-0.828468	-3.425492	-1.319890
H	-0.407179	-0.520860	2.207122
H	0.148781	0.589902	1.307820
H	1.269527	-1.993805	3.224918
H	0.343318	-2.365691	2.024277
H	2.921629	-3.258253	3.436792
H	3.429327	-2.137933	4.368983
H	3.549717	-2.487044	6.624516
H	4.547878	-3.344347	5.820357
H	-0.794505	-5.076014	1.902126
H	-0.534641	-4.078955	0.755303
H	4.251184	-5.281753	4.808707
H	5.755852	-5.108253	5.012943
H	2.124995	-6.210736	0.925829
H	0.686447	-5.953559	0.448800
H	-0.183545	-3.799017	3.598295
H	0.595951	-5.120966	3.617931
H	4.083504	-3.757271	1.247636
O	4.192014	-2.821569	1.035426
H	3.896438	-2.379868	1.851336

$Cl^- (H_2O)_{14}$

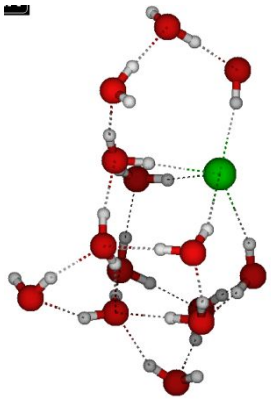


Figure S_{100} : Cl^- optimized structure with 14 water molecules.

E = -1084.861191
H = -1084.860247

O	0.013491	-2.271132	-0.031901
O	2.323851	-2.618092	-1.090199
O	1.427069	-4.889625	-2.214611
O	0.877621	-6.407414	0.014819
O	-1.174698	-4.695072	0.740044
O	-0.612705	-4.555120	3.436387
O	4.063412	-3.305216	0.983524
O	0.451663	-2.011805	2.740566
O	2.963154	-2.609325	3.511679
O	3.579245	-2.665655	6.155397
O	5.571244	-4.481577	6.353042
O	-0.117607	0.239839	1.261966
O	-1.254704	-3.904026	-2.049212
Cl	2.592379	-5.652544	2.866687
H	-0.179705	-1.329019	0.126468
H	0.943700	-2.344559	-0.436930
H	1.357803	-5.517106	-1.461491
H	0.503121	-4.623527	-2.376333

H	3.003220	-2.835303	-0.420019
H	2.130372	-3.457460	-1.582740
H	-1.598204	-4.489523	-1.361973
H	-0.934860	-3.145739	-1.532052
H	0.004997	-0.378678	2.011987
H	0.753371	0.617089	1.117265
H	1.380776	-2.113364	3.058716
H	0.443626	-2.325554	1.815684
H	2.826910	-3.574746	3.421320
H	3.224903	-2.486390	4.453736
H	2.818173	-3.077781	6.570377
H	4.316524	-3.312052	6.266433
H	-1.192173	-4.758340	1.718616
H	-0.787782	-3.818947	0.562253
H	5.396739	-5.233642	5.735976
H	6.392035	-4.086961	6.052361
H	1.480394	-6.374433	0.769581
H	0.100723	-5.878502	0.296153
H	-0.335708	-3.620612	3.392630
H	0.218775	-5.051894	3.423919
H	3.774030	-4.194053	1.235783
H	3.885391	-2.790871	1.787614
H	4.192153	-6.313244	4.158428
O	5.047524	-6.471789	4.613621
H	5.663584	-6.628475	3.894567

$Cl^-(H_2O)_{15}$

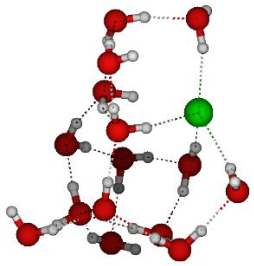


Figure S_{101} : Cl^- optimized structure with 15 water molecules.

E = -1161.275113
H = -1161.274169

O	0.320885	-2.293988	0.154461
O	2.794182	-2.551069	-0.564994
O	2.182286	-4.836199	-1.812291
O	1.362241	-6.393313	0.304523
O	-0.865463	-4.810524	0.546643
O	-1.775119	-4.476051	3.079249
O	4.028591	-3.417891	1.841494
O	-0.019872	-2.198576	2.945653
O	2.396449	-2.854353	3.998301
O	4.485549	-2.459007	5.621053
O	6.071965	-3.600702	3.813760
O	5.645748	-6.308535	4.299708
O	-0.259726	0.127118	1.476760
O	-0.503058	-3.955764	-2.128764
Cl	2.634743	-5.963835	3.468399
H	0.059820	-1.365587	0.296249
H	1.298892	-2.320622	-0.098612
H	2.022634	-5.474544	-1.083002
H	1.285241	-4.614303	-2.127195
H	3.360517	-2.785480	0.191213

H	2.693081	-3.385757	-1.096300
H	-0.927286	-4.533785	-1.476657
H	-0.317171	-3.164732	-1.599394
H	-0.308624	-0.522983	2.207512
H	0.586961	0.563445	1.596487
H	0.811594	-2.321974	3.451137
H	0.202228	-2.455326	2.029256
H	2.347533	-3.829531	4.026046
H	3.068496	-2.604278	4.682092
H	4.497147	-3.060663	6.368414
H	5.165469	-2.820126	4.987927
H	-1.348239	-4.813136	1.407079
H	-0.481062	-3.918328	0.488737
H	6.038684	-4.561235	3.999977
H	5.547195	-3.487821	2.999554
H	1.799526	-6.414935	1.164785
H	0.512585	-5.923498	0.454434
H	-1.275824	-3.652773	3.220531
H	-1.327355	-5.155951	3.618635
H	3.739408	-4.342274	1.867206
H	3.444112	-3.007294	2.515271
H	4.674899	-6.313856	4.179155
H	5.969888	-6.884948	3.603787
H	0.535349	-6.433696	4.140063
O	-0.331888	-6.360043	4.578009
H	-0.117168	-6.030524	5.453319

$Cl^-(H_2O)_{16}$

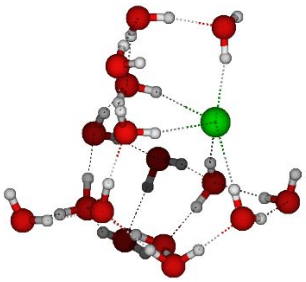


Figure S_{102} : Cl^- optimized structure with 16 water molecules.

E = -1237.691125
H = -1237.690181

O	0.334936	-2.425108	0.194309
O	2.761914	-2.954295	-0.553517
O	1.960588	-5.386561	-1.421000
O	1.096787	-6.473885	1.056598
O	-0.937726	-4.760950	0.938062
O	-1.658179	-4.264958	3.450247
O	-0.186001	-6.237485	4.672536
O	0.138048	-2.014718	3.012561
O	2.623935	-2.531893	3.979623
O	4.713368	-1.822069	5.478059
O	6.317545	-3.109769	3.783584
O	-0.082982	0.120989	1.285563
O	4.220780	-3.297971	1.857444
O	5.967330	-5.752939	4.573004
O	-0.626953	-4.339949	-1.831157
Cl	2.945099	-5.700567	3.664691
H	0.141319	-1.471792	0.270902
H	1.297985	-2.545705	-0.076605
H	1.767659	-5.919128	-0.626659
H	1.077814	-5.121821	-1.747832

H	3.389934	-3.047649	0.184809
H	2.612797	-3.861157	-0.921245
H	-1.073495	-4.774988	-1.088774
H	-0.391303	-3.482211	-1.445373
H	-0.128441	-0.435758	2.090682
H	0.762870	0.570664	1.346665
H	0.995347	-2.087262	3.484174
H	0.306394	-2.393285	2.130367
H	2.602183	-3.493629	4.135958
H	3.294799	-2.171168	4.614471
H	4.779966	-2.300639	6.306996
H	5.400550	-2.228745	4.882891
H	-1.368716	-4.658494	1.828394
H	-0.549074	-3.886544	0.746008
H	6.311978	-4.042254	4.081724
H	5.780258	-3.110105	2.970345
H	1.713882	-6.122958	1.719391
H	0.319221	-5.851662	1.050359
H	-1.146093	-3.444961	3.545172
H	-1.176838	-4.954106	3.961769
H	4.001425	-4.218239	2.076404
H	3.640574	-2.810683	2.481555
H	5.001058	-5.826517	4.443708
H	6.335069	-6.399305	3.966070
H	-0.181338	-7.037702	4.108717
H	0.743284	-5.969775	4.664930
H	1.276468	-8.495137	3.300746
O	0.394392	-8.360920	2.942561
H	0.555345	-7.817699	2.140337

$Cl^-(H_2O)_{17}$

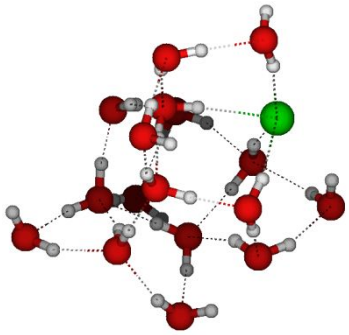


Figure S_{103} : Cl^- optimized structure with 17 water molecules.

E = -1314.103624
H = -1314.102680

O	0.405445	-2.460048	0.282663
O	2.807184	-3.064503	-0.363884
O	1.948582	-5.396432	-1.491946
O	-0.610078	-4.769943	1.323752
O	-2.013804	-3.756781	3.419629
O	1.214795	-6.837750	0.902187
O	-0.165449	-5.802174	4.093558
O	0.689194	-8.270935	3.299637
O	0.032010	0.127241	1.259454
O	0.122607	-1.913985	3.102657
O	2.445912	-2.587593	4.225067
O	4.689746	-1.695183	5.424189
O	6.171667	-3.041802	3.662081
O	3.893408	-3.580635	2.128209
O	6.526373	-5.783778	4.117138
O	-0.652091	-4.320681	-1.605893
Cl	3.589987	-6.611632	3.171666

H	0.218797	-1.502892	0.349098
H	1.378430	-2.599750	0.022520
H	1.799257	-6.062131	-0.799255
H	1.050448	-5.094091	-1.730571
H	3.305946	-3.247146	0.458706
H	2.656253	-3.930491	-0.812142
H	-1.022846	-4.806661	-0.858208
H	-0.386300	-3.481938	-1.190582
H	-0.044838	-0.360015	2.105273
H	0.890241	0.555829	1.298521
H	0.947229	-2.033576	3.636477
H	0.337739	-2.313109	2.241935
H	2.281957	-3.420543	4.747663
H	3.171469	-2.112133	4.699122
H	4.772562	-2.165286	6.256792
H	5.330290	-2.144171	4.808210
H	-1.325585	-4.497189	1.945046
H	-0.237537	-3.925633	0.993519
H	6.379355	-3.960058	3.925238
H	5.503899	-3.148097	2.956689
H	2.002058	-6.633143	1.436184
H	0.562809	-6.131469	1.083206
H	-1.382431	-3.015534	3.501558
H	-1.686076	-4.439153	4.023899
H	3.844705	-4.537795	2.307293
H	3.314323	-3.178636	2.819956
H	5.626481	-6.133188	3.972704
H	7.024354	-6.123541	3.369828
H	-0.005609	-6.764855	3.949056

H	-0.003535	-5.417266	3.219882
H	1.617385	-8.167497	3.554923
H	0.712221	-8.061348	2.347921
H	2.659713	-5.483395	5.004598
O	2.034846	-4.897537	5.462510
H	1.166507	-5.209361	5.127704

$Cl^-(H_2O)_{18}$

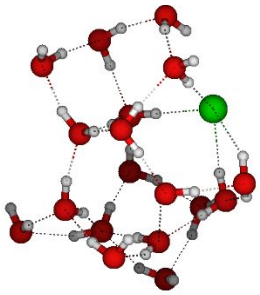


Figure S_{104} : Cl^- optimized structure with 18 water molecules.

E = -1390.512144
H = -1390.511200

O	0.367970	-2.393230	0.295078
O	2.741325	-3.050825	-0.394517
O	1.781388	-5.256041	-1.695216
O	-0.521236	-4.788665	1.291995
O	-1.842884	-3.954725	3.509662
O	3.850735	-3.750570	2.049779
O	2.496243	-2.712456	4.184959
O	1.949404	-4.735768	5.804279
O	0.159114	-1.981821	3.142885
O	4.728037	-1.512319	5.090562
O	6.168628	-2.975186	3.411886
O	0.189455	-5.882125	4.022191

O	0.770135	-8.348081	3.001516
O	0.088139	0.153136	1.408085
O	1.110828	-6.897361	0.592817
O	6.564545	-5.606887	4.279306
O	-0.801649	-4.134767	-1.612563
Cl	3.728059	-6.933177	2.610349
H	0.209905	-1.435966	0.413565
H	1.334224	-2.547342	0.017855
H	1.637331	-5.985245	-1.069132
H	0.883411	-4.914105	-1.872924
H	3.237382	-3.305863	0.410188
H	2.557863	-3.875487	-0.903310
H	-1.126602	-4.673277	-0.880373
H	-0.502806	-3.328011	-1.156222
H	0.010953	-0.374112	2.229634
H	0.961380	0.550019	1.451378
H	1.006219	-2.136542	3.633810
H	0.333002	-2.335191	2.253379
H	2.316556	-3.439209	4.843263
H	3.222251	-2.158191	4.564034
H	4.949177	-1.804245	5.977119
H	5.355976	-1.998777	4.486815
H	-1.199670	-4.578273	1.976519
H	-0.201391	-3.919127	0.977295
H	6.427716	-3.846741	3.771624
H	5.474717	-3.188098	2.757072
H	1.958972	-6.773541	1.051214
H	0.532114	-6.157526	0.872229
H	-1.263789	-3.170601	3.581302

H	-1.416860	-4.634530	4.053587
H	3.841933	-4.719335	2.152190
H	3.292391	-3.401578	2.785729
H	5.860295	-5.811331	4.917699
H	6.295405	-6.095703	3.492726
H	0.285230	-6.837832	3.796632
H	0.340699	-5.437652	3.176616
H	1.732601	-8.277689	3.092869
H	0.646227	-8.119579	2.061884
H	2.722560	-5.321404	5.870585
H	1.294155	-5.219811	5.258408
H	3.953551	-6.688581	4.657850
O	4.183607	-6.460616	5.591407
H	4.206039	-7.297685	6.061583

$Cl^-(H_2O)_{19}$

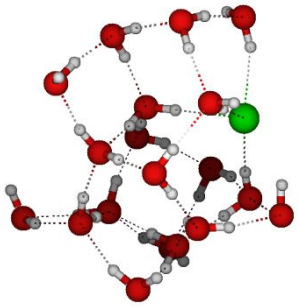


Figure S_{105} : Cl^- optimized structure with 19 water molecules.

E = -1466.922858
H = -1466.921913

O	0.420878	-2.420004	0.259909

O	2.775247	-3.234006	-0.331046
O	1.722584	-5.409969	-1.613242
O	-0.614311	-4.742678	1.301634
O	-1.930871	-3.797205	3.473510
O	0.863800	-6.975286	0.672820
O	3.794302	-3.881910	2.169113
O	2.432089	-2.676072	4.197119
O	1.833674	-4.665070	5.836800
O	0.141453	-1.910283	3.089218
O	4.637850	-1.415270	5.051657
O	6.105261	-3.010853	3.540622
O	0.237804	0.165104	1.286809
O	0.033248	-5.778855	4.066228
O	0.428373	-8.317972	3.124734
O	6.621109	-5.379343	4.818977
O	-0.779393	-4.126664	-1.643412
O	4.051703	-6.412145	5.627820
Cl	3.476219	-7.077427	2.666608
H	0.313134	-1.452193	0.350233
H	1.384780	-2.633949	0.020725
H	1.503035	-6.123120	-0.991342
H	0.857302	-5.010090	-1.829906
H	3.235318	-3.483035	0.496394
H	2.558223	-4.064135	-0.816517
H	-1.174452	-4.632292	-0.922968
H	-0.449901	-3.333532	-1.183035
H	0.104497	-0.327316	2.122710
H	1.124565	0.527451	1.352795
H	0.971146	-2.082232	3.604790

H	0.322209	-2.300316	2.216832
H	2.234936	-3.379470	4.875584
H	3.157019	-2.109147	4.563697
H	4.860397	-1.633013	5.959059
H	5.276835	-1.941667	4.490860
H	-1.292546	-4.481374	1.969122
H	-0.245729	-3.900114	0.968521
H	6.361115	-3.820749	4.037850
H	5.427131	-3.310297	2.906442
H	1.717122	-6.880993	1.127859
H	0.330037	-6.189945	0.917913
H	-1.328862	-3.029204	3.532376
H	-1.534115	-4.472594	4.044355
H	3.711188	-4.840325	2.312739
H	3.238192	-3.457687	2.867841
H	5.791920	-5.669048	5.232040
H	6.764015	-6.008403	4.085195
H	0.067136	-6.744995	3.872642
H	0.199057	-5.371137	3.204762
H	1.390075	-8.344246	3.229616
H	0.335835	-8.101221	2.178194
H	2.596154	-5.265515	5.897072
H	1.163110	-5.135274	5.298355
H	3.838226	-6.672044	4.703016
H	4.073564	-7.233618	6.124691
H	5.730594	-7.252773	2.485272
O	6.677307	-7.030799	2.540899
H	6.814844	-6.413153	1.818019

$Cl^-(H_2O)_{20}$

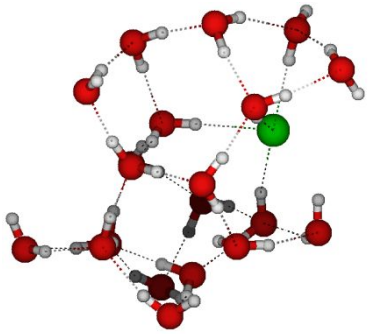


Figure S_{106} : Cl^- optimized structure with 20 water molecules.

E = -1543.331828
H = -1543.330884

O	0.199207	-2.163568	0.385641
O	2.531973	-2.840208	-0.429115
O	1.458005	-4.911691	-1.867293
O	-0.710657	-4.613983	1.228879
O	-1.912322	-3.955931	3.566596
O	0.804536	-6.697672	0.322225
O	3.719614	-3.737235	1.915185
O	2.460752	-2.842232	4.160726

O	1.943093	-4.897898	5.749497
O	0.103690	-1.996365	3.269655
O	4.660891	-1.530675	4.954470
O	6.092842	-2.883035	3.185962
O	6.647206	-5.268021	4.428561
O	0.043743	0.278366	1.724731
O	0.128276	-5.909868	3.906049
O	0.524190	-8.299310	2.631967
O	-1.072847	-3.715094	-1.606502
O	6.468252	-7.670743	2.789444
O	4.217800	-6.436241	5.242984
Cl	3.527539	-6.982978	2.177649
H	0.079692	-1.216381	0.597058
H	1.150298	-2.322552	0.067523
H	1.297554	-5.681140	-1.296523
H	0.570935	-4.518599	-1.987290
H	3.047257	-3.163159	0.337999
H	2.307307	-3.619961	-0.988295
H	-1.396046	-4.300360	-0.910365
H	-0.739551	-2.954739	-1.096750
H	-0.024757	-0.311908	2.503111
H	0.927460	0.650551	1.775214
H	0.964423	-2.214139	3.712899
H	0.235178	-2.276264	2.347748
H	2.308003	-3.582694	4.811291
H	3.186214	-2.273724	4.523788
H	4.972624	-1.822144	5.813781
H	5.278909	-1.955467	4.293844
H	-1.342220	-4.457371	1.970956

H	-0.390858	-3.726117	0.972010
H	6.380735	-3.718948	3.614369
H	5.387255	-3.151281	2.567937
H	1.683114	-6.616243	0.726376
H	0.263346	-5.957796	0.675467
H	-1.324598	-3.181980	3.673085
H	-1.472510	-4.672783	4.048984
H	3.709735	-4.708346	1.939392
H	3.201465	-3.443463	2.704311
H	5.822610	-5.543609	4.871541
H	6.829949	-6.002394	3.824344
H	0.164232	-6.843472	3.591604
H	0.278800	-5.397363	3.101230
H	1.490014	-8.294073	2.694025
H	0.380971	-7.979491	1.721248
H	2.715443	-5.489058	5.794370
H	1.276946	-5.362147	5.203838
H	3.905297	-6.500867	4.321391
H	4.540862	-7.342034	5.425404
H	5.590185	-7.442911	2.410516
H	7.017497	-7.943797	2.051616
H	4.602295	-9.449273	4.509136
O	5.302975	-8.975338	4.964794
H	5.878449	-8.646673	4.248103

$SO_4^{2-}(H_2O)$

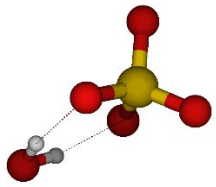


Figure S_{107} : SO_4^{2-} optimized structure with 1 water molecule.

E = -387.174602
H = -387.173658

O	-0.011497	0.913308	0.955240
S	0.243534	-0.321224	-0.118124
O	-0.338896	-1.710314	0.506555
O	1.839495	-0.447506	-0.427575
O	-0.561690	0.029942	-1.521571
H	-1.418389	1.654707	-1.229668
O	-1.650355	2.434814	-0.678348
H	-1.125181	2.122782	0.091877

$SO_4^{2-}(H_2O)_2$

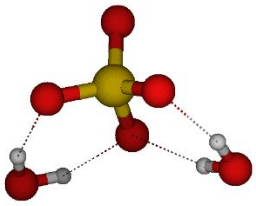


Figure S_{108} : SO_4^{2-} optimized structure with 2 water molecules.

E = -463.608381
H = -463.607437

O	-1.782424	1.791466	-1.034916
O	0.190991	1.199170	0.845337
S	0.502996	-0.330518	0.335935
O	-0.645083	-0.751386	-0.794288
O	0.373662	-1.357349	1.610798
O	1.977995	-0.424247	-0.329643
H	-1.591661	0.844447	-1.193086
H	-1.134601	1.881614	-0.305369
H	-0.803443	-2.723416	1.074061
O	-1.426490	-3.136250	0.440160
H	-1.356717	-2.415558	-0.218563

$SO_4^{2-}(H_2O)_3$

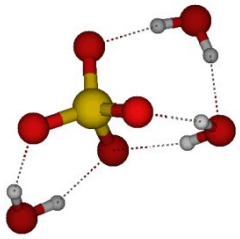


Figure S_{109} : SO_4^{2-} optimized structure with 3 water molecules.

E = -540.037038
H = -540.036094

O	-2.059730	1.714943	-0.866470
O	0.143025	1.428419	0.863504
S	0.629545	-0.028279	0.325415
O	2.147825	0.052881	-0.263863
O	-0.389689	-0.531946	-0.887019
O	0.547910	-1.135435	1.533298
O	0.085611	-3.174763	-0.278531
H	-1.682458	0.847213	-1.112454

H	-1.405046	1.902643	-0.166182
H	0.303371	-2.709222	0.559460
H	-0.214379	-2.372027	-0.760972
H	2.674411	-1.633034	-0.930369
O	2.801557	-2.562290	-1.214444
H	1.941826	-2.942794	-0.964910

$SO_4^{2-}(H_2O)_4$

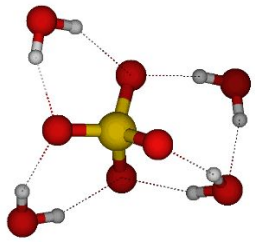


Figure S_{110} : SO_4^{2-} optimized structure with 4 water molecules.

E = -616.462460
H = -616.461516

O	-1.340809	1.992739	-0.502597
O	-0.211512	-0.554310	-0.913611
S	0.966065	-0.433482	0.234973
O	0.631347	-1.485809	1.435712
O	1.007788	1.098262	0.809933
O	2.408908	-0.795651	-0.451917
O	-0.523073	-3.262815	-0.377234
O	2.190599	-3.474006	-1.478883
H	-1.198457	1.095708	-0.858638
H	-0.568317	1.992038	0.091117
H	-0.135493	-2.915144	0.453371
H	-0.603142	-2.398883	-0.833682
H	2.375877	-2.562168	-1.180298

H	1.272922	-3.583415	-1.177331
H	3.637213	0.635605	0.046637
O	3.792905	1.497687	0.473269
H	2.868417	1.652619	0.739722

$SO_4^{2-}(H_2O)_5$

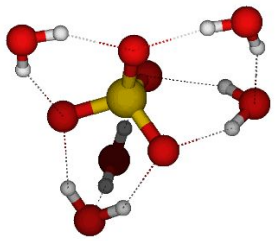


Figure S_{111} : SO_4^{2-} optimized structure with 5 water molecules.

E = -692.885106
H = -692.884161

O	-1.749184	1.810120	-0.963131
O	0.378635	-0.136952	-1.393210
S	1.272018	-0.104398	-0.020322
O	2.630182	-0.978719	-0.202523
O	0.355131	-0.735895	1.196344
O	1.652838	1.439290	0.362552
O	-0.753244	-2.602258	-0.559042
O	4.469210	1.176611	0.165029
O	1.926724	-3.721017	-0.775923
H	-1.044102	1.195286	-1.237347
H	-1.560988	1.904097	-0.014381
H	-0.500020	-2.157389	0.275904
H	-0.520151	-1.874009	-1.166120
H	2.289146	-2.835493	-0.587971
H	0.972409	-3.537077	-0.744683

H	4.155838	0.272877	-0.009490
H	3.591457	1.580191	0.286297
H	0.157280	2.003397	1.341941
O	-0.694747	1.802539	1.781200
H	-0.598927	0.829284	1.785783

$SO_4^{2-}(H_2O)_6$

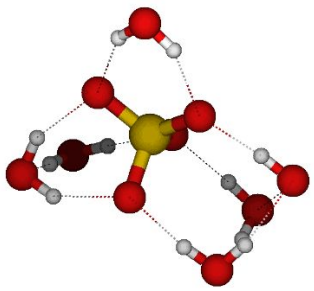


Figure S_{112} : SO_4^{2-} optimized structure with 6 water molecules.

E = -769.611021
H = -769.310077

O	-1.880290	1.684324	-0.987246
O	0.286346	-0.297684	-1.049698
S	1.279834	0.135184	0.172954
O	1.670180	1.710823	0.039196
O	2.633415	-0.771849	0.141155
O	0.502391	-0.090058	1.603018
O	-0.553019	2.517344	1.500006
O	-0.481237	-2.955151	-0.748390
O	4.491359	1.379283	-0.120175
O	2.130762	-3.479334	0.240383
H	-1.197084	1.008081	-1.139896

H	-1.593607	2.063228	-0.139755
H	-0.599948	-2.935849	0.219837
H	-0.254702	-2.019550	-0.949754
H	2.403344	-2.534147	0.214810
H	1.328399	-3.471125	-0.315631
H	4.168301	0.466868	-0.033180
H	3.621565	1.814210	-0.101009
H	0.254028	2.568228	0.949617
H	-0.446033	1.592650	1.794785
H	0.163807	-1.800204	1.973868
O	0.039181	-2.773463	2.057338
H	0.866404	-3.124880	1.678501

$SO_4^{2-}(H_2O)_7$

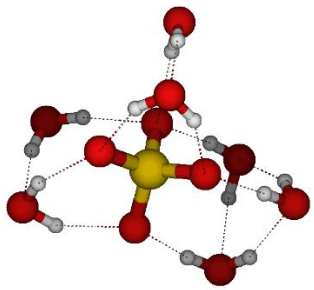


Figure S_{113} : SO_4^{2-} optimized structure with 7 water molecules.

E = -845.729704
H = -845.728760

O	-2.156669	1.543773	-0.563382
O	0.128841	-0.368340	-0.922075
S	1.151903	0.098254	0.272699
O	0.429341	-0.106123	1.719514
O	1.525139	1.673080	0.081512
O	2.521680	-0.783066	0.198968

O	2.071750	-3.500176	0.493225
O	0.020863	-2.777768	2.327479
O	-0.570864	2.527913	1.701152
O	-0.569596	-3.063668	-0.454010
O	3.755363	1.105995	-1.490126
H	-1.478328	0.892434	-0.804144
H	-1.762381	1.974200	0.213228
H	-0.665322	-3.000073	0.514566
H	-0.382478	-2.138139	-0.716419
H	2.334768	-2.558493	0.401319
H	1.262499	-3.536876	-0.051561
H	3.636658	0.270837	-1.001078
H	3.055157	1.621438	-1.044423
H	0.185459	2.566035	1.083617
H	-0.451776	1.607423	1.999895
H	0.123405	-1.809854	2.197315
H	0.842946	-3.130191	1.936879
H	1.089319	0.000473	-2.682865
O	1.709874	0.217362	-3.397187
H	2.482080	0.542962	-2.905977

$SO_4^{2-}(H_2O)_8$

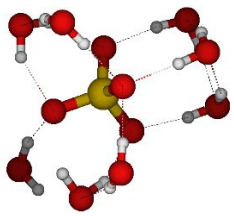


Figure S_{114} : SO_4^{2-} optimized structure with 8 water molecules.

E = -922.143370
H = -922.142426

O	-2.368450	1.347915	-0.817998
O	-1.132260	2.260695	1.666112
O	1.268903	1.632361	0.324245
S	0.936140	0.027672	0.371987
O	2.351108	-0.781433	0.362403
O	0.064185	-0.382151	-0.950066
O	0.091801	-0.296466	1.720027
O	1.996061	-3.539709	0.474995
O	-0.246413	-3.029309	2.137001
O	3.646316	1.178676	-1.109502
O	-0.557930	-3.146696	-0.696095
O	1.804628	0.217732	-3.273139
H	-1.621639	0.755822	-0.999139
H	-2.112397	1.744902	0.030757
H	-0.746815	-3.149802	0.261037
H	-0.401109	-2.200909	-0.889474
H	2.233606	-2.588877	0.462449
H	1.246664	-3.571112	-0.149873
H	3.458319	0.340477	-0.636857
H	2.836896	1.665878	-0.867596
H	-0.313758	2.407313	1.158220
H	-0.965939	1.343281	1.947929
H	-0.175030	-2.053436	2.087294
H	0.626181	-3.322189	1.811585
H	1.143231	-0.004004	-2.596786
H	2.554409	0.519615	-2.741445
H	2.812580	2.335277	1.411983
O	3.730029	2.646314	1.480657

H	4.116956	2.210896	0.710029

$SO_4^{2-}(H_2O)_9$

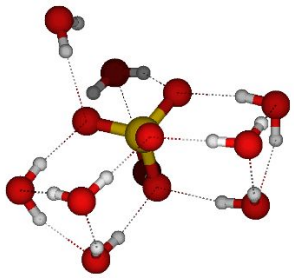


Figure S_{115} : SO_4^{2-} optimized structure with 9 water molecules.

E = -998.565035
H = -998.564091

O	-1.971035	1.563622	-0.940531
O	-1.702850	1.862697	1.879955
O	1.756566	1.618764	0.241682
S	1.186229	0.089879	0.339498
O	0.313963	-0.098485	1.691390
O	2.461410	-0.916240	0.327282
O	0.244721	-0.215500	-0.968927
O	4.052574	0.770212	-1.176290
O	1.822817	-3.614755	0.471372
O	-0.332441	-2.803954	2.116862
O	-0.657471	-2.916237	-0.711933
O	4.347790	2.233539	1.419394
O	2.070237	0.040653	-3.309757
H	-1.243440	0.922940	-1.064185
H	-2.141386	1.519998	0.019320
H	-0.843911	-2.888275	0.245507
H	-0.390188	-1.998593	-0.913884

H	2.161195	-2.695868	0.451639
H	1.079062	-3.568388	-0.158886
H	3.725557	-0.010501	-0.681753
H	3.338050	1.393304	-0.954703
H	-1.200752	2.614340	1.510600
H	-1.032264	1.152611	1.922517
H	-0.142141	-1.845642	2.078368
H	0.498790	-3.204119	1.796943
H	1.387355	-0.068577	-2.628449
H	2.860917	0.237583	-2.788126
H	3.390685	2.090119	1.349276
H	4.658250	1.731187	0.655280
H	0.520897	2.962875	0.174591
O	-0.259959	3.550737	0.124057
H	-0.848950	3.061389	-0.481403

$SO_4^{2-}(H_2O)_{10}$

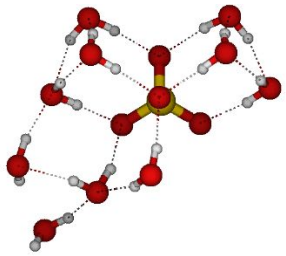


Figure S_{116} : SO_4^{2-} optimized structure with 10 water molecules.

E = -1074.974805
H = -1074.973861

O	-1.448402	1.318643	-0.825433

O	0.285700	2.813799	0.700206
O	2.266524	4.277933	-0.508776
S	1.019519	-0.842343	0.757062
O	0.400557	-0.802433	-0.771573
O	-0.221065	-0.974874	1.805781
O	2.052746	-2.052304	0.927312
O	3.506740	1.706324	-0.655959
O	0.960456	-4.566977	0.418506
O	-1.375566	-3.519400	1.644698
O	-1.847730	1.233771	1.978278
O	-0.988551	-3.253274	-1.165148
O	4.986415	3.663295	0.519041
O	2.497976	-0.182145	-2.742717
H	-0.841430	0.553806	-0.920270
H	-1.872554	1.168421	0.040099
H	-1.402809	-3.293208	-0.282595
H	-0.518631	-2.395804	-1.150847
H	1.444790	-3.741850	0.628011
H	0.415044	-4.294261	-0.343806
H	2.951857	1.162995	-0.037665
H	2.927657	2.452035	-0.898860
H	-1.197511	1.945918	1.884607
H	-1.289505	0.423996	2.001401
H	-1.024271	-2.617219	1.792858
H	-0.570329	-4.039939	1.461788
H	1.784945	-0.492412	-2.160451
H	2.998318	0.413655	-2.168395
H	5.230736	4.047815	-0.326174
H	4.575640	2.808188	0.246921

H	1.496567	3.875111	-0.044037
H	-0.303846	2.472841	-0.011375
H	2.986285	4.285490	0.137364
O	1.771994	0.588112	1.027475
H	0.825988	2.012951	0.914259

$SO_4^{2-}(H_2O)_{11}$

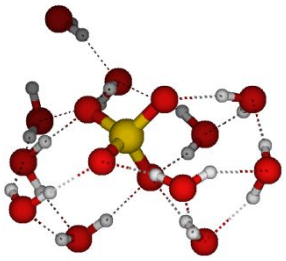


Figure S_{117} : SO_4^{2-} optimized structure with 11 water molecules.

E = -1151.391191
H = -1151.390247

O	-1.439600	1.255698	-0.921862
O	0.159379	2.990941	0.483116
O	1.536713	0.848644	1.378635
S	0.861624	-0.636745	1.201893
O	1.907766	-1.763209	1.634944
O	0.435405	-0.776905	-0.393092
O	-0.487623	-0.753334	2.090687
O	3.460951	1.444803	-0.388311
O	4.929552	3.611066	0.381783
O	2.301660	3.968938	-0.943467
O	-2.090603	1.468724	1.822212
O	0.753639	-4.820912	-0.051277
O	-1.047852	-3.617478	1.880884

O	-1.271439	-3.006128	-0.865848
O	2.756806	-0.989342	-1.902170
H	-0.813155	0.504970	-0.852919
H	-1.947324	1.201025	-0.090623
H	-1.504189	-3.192752	0.063316
H	-0.710828	-2.210857	-0.784297
H	1.607916	-4.359974	-0.178777
H	0.113904	-4.293216	-0.564032
H	2.840649	1.124328	0.317510
H	2.939719	2.127762	-0.852691
H	-1.427876	2.165981	1.721404
H	-1.555877	0.662633	2.003275
H	-0.783493	-2.705093	2.095114
H	-0.260778	-4.037639	1.485603
H	1.872984	-0.944524	-1.481512
H	3.216157	-0.238871	-1.492289
H	5.269996	3.768217	-0.502099
H	4.516200	2.720156	0.292862
H	1.488068	3.748218	-0.432730
H	-0.390986	2.532811	-0.193447
H	2.986077	4.146490	-0.283118
H	0.651664	2.235680	0.886952
H	2.788237	-2.777422	0.467819
O	3.132187	-3.295712	-0.287041
H	3.115852	-2.627527	-0.998369

$SO_4^{2-}(H_2O)_{12}$

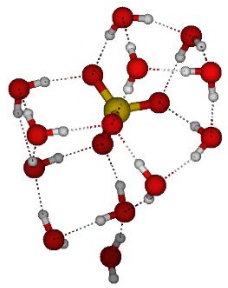


Figure S_{118} : SO_4^{2-} optimized structure with 12 water molecules.

E = -1227.817332
H = -1227.816388

O	-1.455601	1.311474	-0.922607
O	0.194336	3.011425	0.467579
O	1.575818	0.834777	1.309777
S	0.821236	-0.610577	1.173881
O	-0.505689	-0.619685	2.099897
O	1.830831	-1.788513	1.601613
O	0.366159	-0.780570	-0.403107
O	3.447508	1.510008	-0.485587
O	4.940514	3.642076	0.360963
O	3.290614	-3.045774	-0.459454
O	-2.075630	1.638259	1.817939
O	2.316855	4.048423	-0.934360
O	2.647785	-0.814654	-2.029927
O	1.247677	-4.970608	-0.344116
O	-0.946053	-3.301846	-0.744160
O	-1.643952	-3.246656	1.954448
H	-0.865691	0.532541	-0.854644
H	-1.957534	1.293557	-0.086368
H	-1.344729	-3.352369	0.151463
H	-0.508437	-2.431179	-0.733816

H	2.008271	-4.371458	-0.498322
H	0.460946	-4.440719	-0.600761
H	2.847580	1.157857	0.220701
H	2.928562	2.230149	-0.896012
H	-1.400829	2.319473	1.684313
H	-1.551650	0.831254	2.013768
H	-1.365232	-2.319614	2.069932
H	-0.837006	-3.753136	2.199256
H	1.783139	-0.814895	-1.572144
H	3.104393	-0.056731	-1.627614
H	5.301603	3.821537	-0.510360
H	4.530463	2.754585	0.241949
H	1.507103	3.818659	-0.422249
H	-0.360382	2.561737	-0.211455
H	3.008265	4.215259	-0.278057
H	0.686561	2.252805	0.862280
H	2.898868	-2.603785	0.316442
H	3.180226	-2.367947	-1.155447
H	1.222893	-3.446502	2.245642
O	0.860616	-4.347622	2.324441
H	1.018233	-4.718767	1.425352

$SO_4^{2-}(H_2O)_{13}$

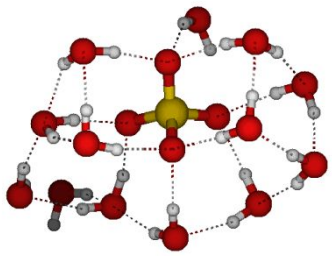


Figure S_{119} : SO_4^{2-} optimized structure with 13 water molecules.

E = -1304.225205
H = -1304.224260

O	-1.380228	1.385859	-1.300812
O	0.144383	3.097572	0.248338
O	1.462385	0.894344	1.081299
S	0.736035	-0.562618	1.025633
O	0.253683	-0.835841	-0.515531
O	-0.569846	-0.556454	1.996515
O	1.782300	-1.690274	1.520712
O	3.456964	1.495827	-0.596316
O	4.912682	3.444976	0.697166
O	2.481224	4.113219	-0.830446
O	-2.204507	1.634366	1.369188
O	2.514967	-0.726928	-2.221497
O	3.157106	-2.958962	-0.647234
O	1.203011	-4.959285	-0.437476
O	1.109427	-4.379099	2.252382
O	-1.447623	-3.334349	2.201721
O	-1.084675	-3.382796	-0.557457
H	-0.829156	0.589312	-1.179608
H	-1.947236	1.378342	-0.505804
H	-1.360918	-3.431995	0.383605
H	-0.680289	-2.500339	-0.628053
H	1.918491	-4.323453	-0.648261
H	0.370488	-4.461108	-0.593790
H	2.805254	1.159045	0.067401
H	3.024737	2.297255	-0.955796

H	-1.534942	2.332453	1.328900
H	-1.701553	0.843247	1.654684
H	-1.212043	-2.392986	2.261712
H	-0.599001	-3.807017	2.357405
H	1.658527	-0.748430	-1.754085
H	2.986727	0.011851	-1.800086
H	5.438698	3.690223	-0.067398
H	4.507189	2.594922	0.415486
H	1.606131	3.902735	-0.433500
H	-0.336808	2.665855	-0.492732
H	3.104424	4.178823	-0.091967
H	0.598725	2.327985	0.662659
H	2.803367	-2.518105	0.145173
H	3.036982	-2.280425	-1.340437
H	1.415238	-3.464508	2.137172
H	1.170447	-4.742993	1.337930
H	0.289054	-0.690513	3.825603
O	1.035457	-0.919333	4.398551
H	1.661303	-1.251313	3.744010

$SO_4^{2-}(H_2O)_{14}$

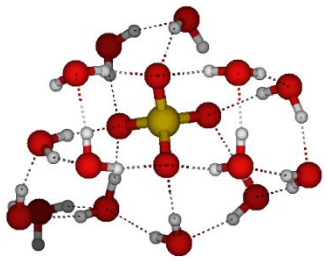


Figure S_{120} : SO_4^{2-} optimized structure with 14 water molecules.

E = -1380.640360
H = -1380.639415

O	-1.440615	1.319131	-0.926902
O	0.186164	2.869045	0.648291
O	1.556446	0.591497	1.431159
S	0.784522	-0.813825	1.105456
O	1.743693	-2.060676	1.485479
O	0.395547	-0.815767	-0.478795
O	-0.575814	-0.905357	1.997091
O	3.463112	1.425532	-0.351964
O	4.974820	3.594356	0.442836
O	2.314045	3.924227	-0.732982
O	-2.155373	1.376303	1.784813
O	2.749850	-0.750566	-2.059052
O	3.252474	-3.134560	-0.708129
O	1.173736	-4.973732	-1.084528
O	0.564430	-4.697862	1.572027
O	-1.859365	-3.454368	1.228323
O	-0.939242	-3.185710	-1.384146
O	2.252040	0.775807	4.332737
H	-0.863805	0.532435	-0.909888
H	-1.973883	1.232616	-0.113572
H	-1.426507	-3.349667	-0.548364
H	-0.470363	-2.357061	-1.187772
H	1.957643	-4.384215	-1.074537
H	0.423059	-4.389818	-1.329164
H	2.882196	1.033103	0.338455
H	2.937909	2.171283	-0.713163
H	-1.485642	2.074561	1.780306
H	-1.642263	0.559874	1.955113

H	-1.581512	-2.571543	1.522314
H	-1.084782	-4.021836	1.447724
H	1.864930	-0.764550	-1.651188
H	3.190206	-0.019244	-1.591158
H	5.297551	3.759336	-0.446290
H	4.588952	2.695292	0.366329
H	1.510261	3.710652	-0.206677
H	-0.354257	2.469405	-0.072504
H	3.012239	4.135379	-0.096495
H	0.665638	2.094772	1.012345
H	2.859200	-2.781962	0.108180
H	3.208494	-2.366866	-1.313635
H	0.994188	-3.831326	1.659891
H	0.790520	-4.960536	0.647929
H	2.132778	0.827518	3.374263
H	1.820736	-0.068625	4.542224
H	1.499005	-2.111306	3.618058
O	0.913373	-1.774632	4.311140
H	0.164443	-1.464995	3.775718

$SO_4^{2-}(H_2O)_{15}$

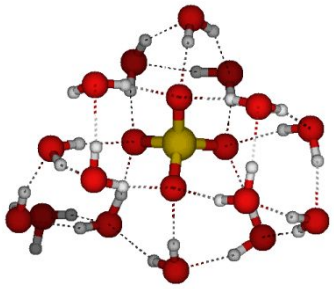


Figure S_{121} : SO_4^{2-} optimized structure with 15 water molecules.

E = -1457.059131

H = -1457.058186

O	-1.429150	1.343053	-0.938344
O	0.218253	2.781908	0.711426
O	2.337872	3.891756	-0.642580
O	1.591991	0.472708	1.420126
S	0.802361	-0.913842	1.035058
O	-0.530738	-1.035333	1.956296
O	1.780046	-2.173833	1.300951
O	0.375943	-0.821076	-0.531711
O	3.456738	1.370024	-0.396536
O	4.997475	3.484071	0.495408
O	-2.139961	1.267661	1.767001
O	2.667127	-0.694821	-2.204842
O	3.171252	-3.169313	-1.031415
O	1.038810	-4.952658	-1.384693
O	0.518943	-4.808209	1.301066
O	-1.883275	-3.516620	1.077235
O	-1.047016	-3.114465	-1.539594
O	0.246253	-1.271042	4.731032
O	2.282799	0.598935	4.185352
H	-0.861409	0.550345	-0.946082
H	-1.971004	1.225774	-0.134685
H	-1.508983	-3.313134	-0.696290
H	-0.550258	-2.310368	-1.316308
H	1.833204	-4.378232	-1.391227
H	0.289468	-4.349099	-1.580264
H	2.886525	0.956992	0.289133
H	2.938312	2.141805	-0.711499

H	-1.462322	1.957960	1.794496
H	-1.640341	0.441200	1.917077
H	-1.590300	-2.659699	1.425556
H	-1.111824	-4.105907	1.247702
H	1.798769	-0.723887	-1.764979
H	3.135095	-0.000244	-1.708748
H	5.338650	3.690094	-0.378100
H	4.607086	2.592898	0.369446
H	1.539258	3.665403	-0.114796
H	-0.328182	2.424691	-0.027524
H	3.047505	4.071043	-0.008648
H	0.697964	1.989394	1.031650
H	2.822364	-2.860246	-0.179545
H	3.120364	-2.364588	-1.585962
H	0.983358	-3.969019	1.445944
H	0.720966	-5.016087	0.357296
H	2.105722	0.656999	3.229986
H	1.469221	0.186091	4.534259
H	1.033570	-1.837107	4.614659
H	-0.141137	-1.236400	3.839604
H	2.577814	-2.252997	3.051104
O	2.823148	-2.158944	3.987306
H	2.943373	-1.195796	4.092374

$SO_4^{2-}(H_2O)_{16}$

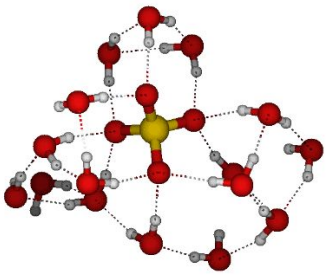


Figure S_{122} : SO_4^{2-} optimized structure with 16 water molecules.

E = -1533.464941
H = -1533.463997

O	-1.341994	1.607077	-1.074981
O	0.253975	3.046856	0.645428
O	2.595209	3.947317	-0.516087
O	3.411223	1.299864	-0.350341
O	1.425276	0.685446	1.453703
S	0.594101	-0.691849	1.133249
O	0.217182	-0.700685	-0.451851
O	-0.776398	-0.731266	2.003184
O	1.491013	-1.965802	1.525355
O	5.106421	3.174041	0.768754
O	-2.249638	1.628230	1.567077
O	2.401151	-0.626665	-2.225898
O	3.254059	-3.222952	-2.558040
O	1.199763	-4.833042	-1.462824
O	1.081110	-5.533556	1.468376
O	-1.183041	-3.820940	1.729536
O	-0.946681	-3.275860	-0.969965
O	1.978305	0.736362	4.286679
O	2.139949	-2.083267	4.289893
O	-0.317194	-0.824500	4.807540

H	-0.826999	0.781070	-1.012552
H	-1.943358	1.550240	-0.307934
H	-1.179976	-3.523036	-0.047416
H	-0.603206	-2.369358	-0.882025
H	1.781468	-4.368979	-2.096840
H	0.391954	-4.268242	-1.360508
H	2.779622	0.970214	0.327221
H	3.007911	2.138199	-0.662164
H	-1.538974	2.280777	1.636607
H	-1.814811	0.778318	1.781202
H	-0.958697	-2.926244	2.020573
H	-0.364057	-4.348464	1.805907
H	1.591534	-0.673900	-1.685091
H	2.964554	-0.017006	-1.719440
H	5.555874	3.390460	-0.051473
H	4.638378	2.340613	0.546618
H	1.737445	3.797726	-0.060037
H	-0.251128	2.700447	-0.126032
H	3.273265	4.000540	0.173476
H	0.657199	2.234302	1.017146
H	3.591750	-3.352660	-1.658999
H	2.953671	-2.286942	-2.545586
H	1.895910	-5.009805	1.521547
H	0.988480	-5.642526	0.511197
H	1.879428	0.805756	3.321498
H	1.094073	0.449252	4.585844
H	0.400586	-1.487706	4.789525
H	-0.605783	-0.795786	3.878176
H	1.970731	-2.174274	3.335313

H	2.401141	-1.146553	4.368197
H	2.684960	-3.006837	0.642869
O	3.094299	-3.823170	0.299522
H	2.390517	-4.191529	-0.275030

$SO_4^{2-}(H_2O)_{17}$

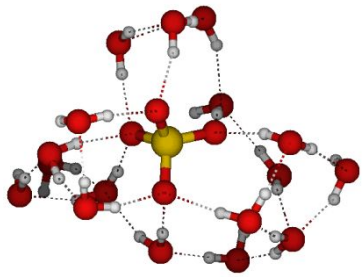


Figure S_{123} : SO_4^{2-} optimized structure with 17 water molecules.

E = -1609.871986
H = -1609.871042

O	-1.424496	1.869140	-1.004714
O	0.441264	3.010838	0.637530
O	1.399746	0.469172	1.429220
S	0.185318	-0.623544	1.178313
O	0.721337	-2.097858	1.573357
O	-0.206799	-0.599089	-0.399324
O	-1.061697	-0.228353	2.114024
O	3.285524	-4.228470	0.376219
O	3.298867	1.160325	-0.408777
O	5.280476	2.867860	0.470763
O	2.722430	3.832021	-0.619321
O	1.172842	-4.684602	-1.625221
O	-1.100605	-3.267637	-1.183522
O	-0.899232	-4.411599	1.330179

O	-2.259426	2.231453	1.630448
O	2.080249	-0.611024	-2.174290
O	3.289872	-3.046936	-2.308806
O	2.278283	-1.624083	5.128463
O	-0.409251	-0.611059	4.891268
O	1.784974	0.988212	4.238631
O	1.137477	-6.280543	0.578046
H	-1.078625	0.959211	-0.931666
H	-2.010849	1.957438	-0.228382
H	-1.217250	-3.710446	-0.314186
H	-0.853924	-2.355155	-0.957274
H	1.877155	-4.175041	-2.078405
H	0.363069	-4.121430	-1.589999
H	2.652553	0.834763	0.258352
H	2.959905	2.040572	-0.687615
H	-1.449750	2.761579	1.646875
H	-1.941854	1.338023	1.870994
H	-0.393375	-3.619773	1.581508
H	-0.231671	-5.108437	1.175929
H	1.277186	-0.633998	-1.624621
H	2.652031	0.038547	-1.726518
H	5.637461	3.022806	-0.406996
H	4.704919	2.086373	0.334941
H	1.884951	3.725890	-0.112342
H	-0.137083	2.710493	-0.104745
H	3.441232	3.877535	0.026839
H	0.767549	2.173442	1.023995
H	3.631918	-3.221118	-1.419984
H	2.868368	-2.156106	-2.275636

H	1.973696	-5.927480	0.908839
H	1.118251	-5.904628	-0.328855
H	1.714314	0.856749	3.276878
H	0.904657	0.712599	4.562707
H	0.329299	-1.240851	4.971229
H	-0.704579	-0.655054	3.965595
H	2.629890	-2.066380	4.339136
H	2.342075	-0.674730	4.904068
H	3.294340	-3.591255	1.114403
H	2.419596	-4.147354	-0.054711
H	2.207221	-2.173577	2.177894
O	3.148361	-2.326337	2.465276
H	3.596509	-1.512015	2.219527

$SO_4^{2-}(H_2O)_{18}$

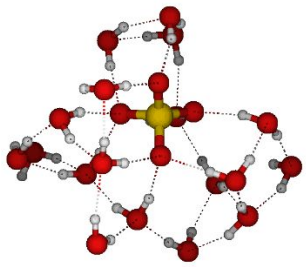


Figure S_{124} : SO_4^{2-} optimized structure with 18 water molecules.

E = -1686.282243
H = -1686.281299

O	-0.500740	1.647566	-1.564160
O	0.776625	2.965359	0.499433
O	3.351619	3.614763	-0.209163
O	3.560687	0.874243	-0.118403
O	1.431422	0.424223	1.518290

S	0.218983	-0.644232	1.170988
O	-1.154258	-0.095184	1.798005
O	0.600477	-2.073693	1.814125
O	0.123840	-0.785743	-0.451221
O	3.067973	-2.244684	2.686935
O	5.509140	2.316056	1.256250
O	-2.098218	2.272780	0.622009
O	2.472046	-0.833276	-2.022382
O	3.751822	-3.302217	-2.224863
O	1.542685	-4.746404	-1.407774
O	-0.789329	-3.411807	-1.239557
O	1.405823	-6.241969	0.855472
O	-0.801357	-4.474332	1.306214
O	3.495079	-4.115780	0.576989
O	-0.854204	-0.433631	4.674545
O	1.421423	1.131561	4.309481
O	1.795438	-1.477483	5.263236
H	-0.310760	0.737951	-1.251550
H	-1.313622	1.884349	-1.075787
H	-0.972041	-3.840740	-0.373587
H	-0.579358	-2.490936	-1.010261
H	2.247178	-4.330500	-1.944404
H	0.714735	-4.212513	-1.489960
H	2.804194	0.652404	0.471616
H	3.399120	1.801765	-0.403478
H	-1.324828	2.805155	0.858525
H	-1.908305	1.413176	1.047099
H	-0.390825	-3.649936	1.618439
H	-0.075511	-5.127383	1.265304

H	1.660385	-0.956847	-1.494568
H	3.007402	-0.223230	-1.475902
H	6.065954	2.500834	0.496200
H	4.916847	1.608715	0.929555
H	2.426078	3.591534	0.117707
H	0.467151	2.608751	-0.363870
H	3.928600	3.535145	0.564017
H	0.960246	2.153506	1.012551
H	4.015701	-3.452992	-1.303574
H	3.346946	-2.409412	-2.229008
H	2.206455	-5.827866	1.203220
H	1.425444	-5.934179	-0.074948
H	1.485332	0.943632	3.357112
H	0.504387	0.865919	4.520673
H	-0.146342	-1.082866	4.832494
H	-1.059799	-0.485107	3.726160
H	2.261166	-1.926254	4.542416
H	1.886722	-0.528826	5.046099
H	3.412861	-3.473695	1.306248
H	2.649233	-4.115358	0.095624
H	2.128605	-2.144719	2.383701
H	3.461381	-1.390112	2.487607
H	1.666963	0.394395	-3.455756
O	1.175129	1.058874	-3.960801
H	0.536117	1.407736	-3.325628