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Theoretical Investigation of the Stepwise Hydrolysis of the $[Re_3(\mu\text{-}Cl)_3Cl_9]^{3-}$ Anion

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A detailed study of the stepwise substitution of the chloride ligands in the $[Re_3(\mu\text{-}Cl)_3Cl_9]^{3-}$ (**1**) anion by water molecules is presented using theoretical methods. Ligand lability as well as the structure and relative stability of the various mono-$[Re_3(\mu\text{-}Cl)_3Cl_8(H_2O)]^{2-}$ (**2a,b**) and dihydro-$[Re_3(\mu\text{-}Cl)_3Cl_7(H_2O)_2]^{-}$ (**3a**–**f**) conformers is examined. Clear preferences for the positions of the incoming water ligands are proposed based on calculated energy and vibrational data, which fully agree with the experimental results.

Introduction

The realization in the early 1960s[1−3] that the polymeric $[Re_3(\mu\text{-}Cl)_3Cl_6]_n$ halide and its related cluster anion **1** contain a 12e$^-$ $[Re_3]^{9+}$ core, with the metal atoms forming between them three double bonds,[4,5] played a key role in the development of the field of metal−metal bonds and transition-metal clusters.[6] This extremely interesting topic of triangulo and higher nuclearity rhenium halide clusters has been recently reviewed by Walton.[7]

Among the wealth of synthetic, crystallographic, and physicochemical studies concerning **1**, a notable exception is the scarcity of theoretical studies. Apart from the original SCF-Xa[8] investigations and a previous study by us,[9] no other theoretical work has, to our knowledge, been applied to this cluster; this with certainty may be attributed to the extremely large size of the calculations involved.

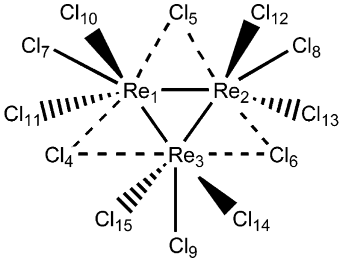

Figure 1. Schematic drawing of the structure of **1**. Cl_{4-6} are bridging, Cl_{7-9} are equatorial, and Cl_{10-15} are axial.

An interesting aspect in the chemistry of **1** (see Figure 1 for labeling of ligands) is the relative lability of terminal in-plane (equatorial), terminal out-of-plane (axial), and bridging halide ligands in halogen exchange and solvolytic reactions. On the basis of halogen, radiochemical ($^{36}Cl^-$), and chloride−pseudohalide (N_3^-, CN^-, and NCS^-) exchange reactions, this was found to be $Cl_{equatorial} > Cl_{axial} \gg Cl_{bridging}$.[10] In a previous work,[9] we examined this from a theoretical point of view and found that ab initio calculations back the experimental findings.[7]

Herein, we address to a more detailed extent the solvolysis of Re−Cl bonds by water molecules, and in a thorough study, using density functional theory (DFT), we investigate the intermediate products in the stepwise displacement of the

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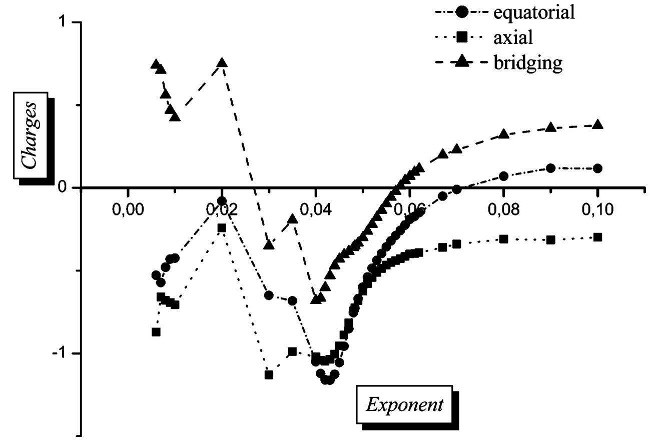

Figure 2. Mulliken charges calculated at the DFT level with various diffuse exponents for the Cl atom.

chloride ligands by water, for the first and second substitution. The total energies of the various positions that water molecules can enter the complex are studied, giving interesting results regarding the relevant activity of the axial and equatorial ligands in the original complex.

Theoretical Details

All calculations were performed using the *Gaussian98* suite of programs[11] at the density functional level of theory with the B3-LYP functional.[12,13] The basis set used is an augmented standard SDD of the above program, which is broken down as follows: For Re atoms, a Stuttgart–Dresden effective core potential is used for the core electrons and 6s5p3d basis functions are used for the outer 15 electrons. An additional f function with exponent 0.5 is added. For Cl atoms, the SDD basis is augmented by diffuse s, p, and d functions with exponents 0.0483, 0.0483, and 0.6, respectively. The exponent of 0.0483 is that of a well-tempered set. We find that the Mulliken partial charges calculated for the Cl atoms are very sensitive to this exponent, as can be seen in Figure 2. It is, however, useful to note that the trend of the axial Cl atoms to always be more negative from the equatorial holds throughout the graph of Figure 2. For O atoms, the same additions were with exponents 0.0845, 0.0845, and 0.850, respectively. Finally, the 2s SDD basis set for H atoms is augmented by s and p functions with exponents 0.0360 and 1.000, respectively.

Results and Discussion

In order to approach the hydrolytic reactivity of this $[Re_3]^{9+}$cluster in a most precise manner, we have performed a wide range of calculations on the parent cluster and the mono- and disubstituted derivatives. The compounds studied are schematically summarized in Figure 3. Complex **1** is unsubstituted, **2** exists in two isomeric forms, depending on the position of the water molecule, either axial (**2a**) or

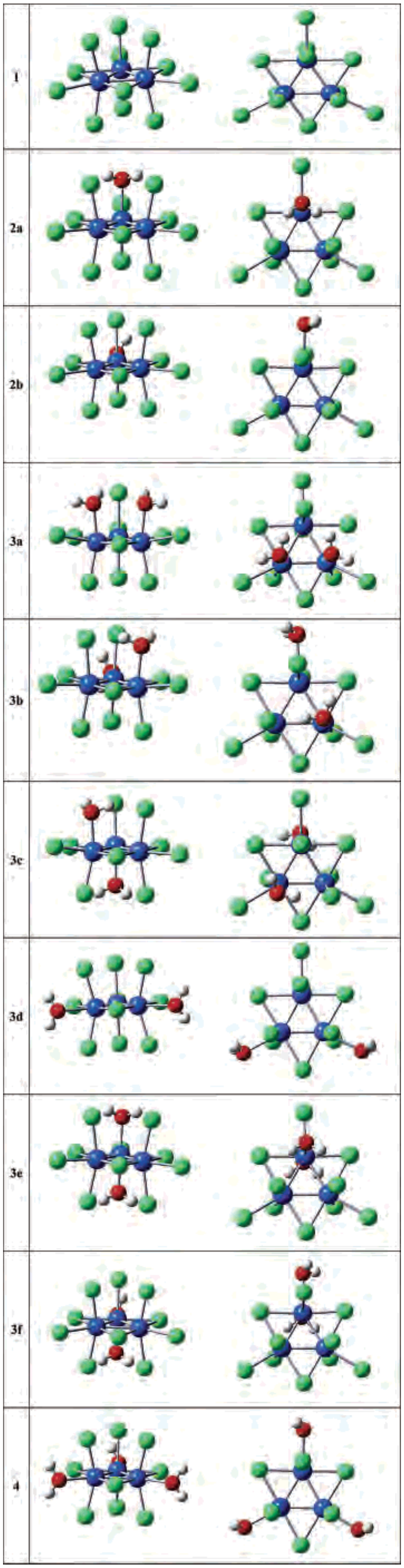

Figure 3. Schematic views from inside and above the Re_3 plane of the complexes **1**, **2a**,**b**, and **3a**–**f** complexes.

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Table 1. Bond Lengths (Å) and Energies (hartrees) of the Complexes As Depicted in Figure 3

	Re−Re	Re−Cl$_{equatorial}$	Re−Cl$_{axial}$	Re−Cl$_{bridging}$	Re−O$_{equatorial}$	Re−O$_{axial}$	energy[a]
$[Re_3(\mu\text{-}\mathbf{Cl})_3Cl_9]^{3-}$ (**1**)	2.469	2.734	2.346	2.464			−5757.904842
$[Re_3(\mu\text{-}\mathbf{Cl})_3Cl_8(H_2O)]^{2-}$ (**2a**)	2.471, 2.481	2.546, 2.591	2.300, 2.416	2.452, 2.471		2.163	−5374.241534
$[Re_3(\mu\text{-}\mathbf{Cl})_3Cl_8(H_2O)]^{2-}$ (**2b**)	2.441, 2.493	2.596, 2.602	2.341, 2.363	2.444, 2.496	2.450		0.013973
$[Re_3(\mu\text{-}\mathbf{Cl})_3Cl_7(H_2O)_2]^{-}$ (**3a**)	2.446, 2.467	2.482, 2.584	2.271, 2.498	2.446, 2.458		2.164, 2.167	−4990.465089
$[Re_3(\mu\text{-}\mathbf{Cl})_3Cl_7(H_2O)_2]^{-}$ (**3b**)	2.438, 2.489	2.471, 2.494	2.287, 2.422	2.438, 2.477	2.505	2.174	0.003394
$[Re_3(\mu\text{-}\mathbf{Cl})_3Cl_7(H_2O)_2]^{-}$ (**3c**)	2.470, 2.479	2.472, 2.498	2.323, 2.376	2.443, 2.462		2.157	0.005369
$[Re_3(\mu\text{-}\mathbf{Cl})_3Cl_7(H_2O)_2]^{-}$ (**3d**)	2.405, 2.459	2.504	2.338, 2.341	2.457, 2.467	2.450		0.005758
$[Re_3(\mu\text{-}\mathbf{Cl})_3Cl_7(H_2O)_2]^{-}$ (**3e**)	2.467, 2.489	2.461, 2.500	2.370	2.440, 2.483		2.100	0.010069
$[Re_3(\mu\text{-}\mathbf{Cl})_3Cl_7(H_2O)_2]^{-}$ (**3f**)	2.435, 2.503	2.494	2.308, 2.423	2.432, 2.442	2.472	2.116	0.017898
$[Re_3(\mu\text{-}\mathbf{Cl})_3Cl_7(H_2O)_3]$ (**4**)	2.424		2.327, 2.328	2.447, 2.467	2.358, 2.361		−4606.593805

[a] The total energy is given for the most stable conformer and energy difference relative to that for the remaining conformers.

equatorial (**2b**). Similarly, **3** exists in six isomeric forms. In **3a** and **3c**, two water molecules are placed in two Re atoms in axial positions cis and trans to the Re_3 plane, respectively; **3b** comprises water molecules in two Re atoms, one in the axial position and one in the equatorial position, and in **3d** in equatorial positions. Finally, **3e** and **3f** correspond to isomers with two water molecules on the same Re atom, either both in the axial position or one in the axial position and one in the equatorial position, respectively. For completeness, a trihydrated complex **4** has also been optimized, however only in the case of all three water molecules in equatorial positions; this is because, as will be seen later, the first two substitutions will be found to be favored in this position.

All structures were optimized in a full and unconstrained manner; i.e., all geometrical parameters (including internal water coordinates) were allowed to vary freely. Minima were reached for all structures, and these were confirmed by a force constant calculation at the equilibrium geometry. A summary of equilibrium bond length data and total energies for all compounds is given in Table 1; these will be discussed in further detail for each particular case.

1. $[Re_3(\mu\text{-Cl})_3Cl_9]^{3-}$ (1). The structure, when optimized, yields a D_{3h} symmetry minimum of the potential energy surface. The calculated bond lengths are generally in good agreement with experimental crystallographic data.[14] In particular, the Re−Re length is found to be 2.469 Å, compared to 2.471 Å found from crystallographic analysis. This excellent agreement is, of course, helped by a cancellation of errors, because calculated results correspond to gas-phase and not vibrationally averaged geometries whereas crystallographic data are solid-state and vibrationally averaged geometries, but in any case shows beyond a doubt that the theoretical approach is accurate.

In agreement with our previous work,[9] it is found that it is not possible to draw definitive conclusions on the relative lability of the chloride ligands of **1** based on Mulliken partial charges alone. Although there is a clear trend favoring the easier removal of the equatorial ligands, when, for example, a diffuse exponent is varied (see Figure 2), further analysis is needed in order to permit the prediction of which chloride ligand would be first removed from this complex.

Conclusions can be drawn from the calculated geometrical data and harmonic vibrational frequencies. The latter for **1** are given in Table 2. The a_1' symmetric vibrations are assigned as follows (full assignments and computed force constants as well as all geometrical data are available from the authors): 138 cm^{-1} Re−Cl in-plane stretch, 192 cm^{-1} Re−Cl in-plane stretch and out-of-plane Re−Cl bend, 253 cm^{-1} Re−Cl out-of-plane stretch and ring breathing, 309 and 338 cm^{-1} Re−Cl bridge stretches, and Re−Cl out-of-plane stretch.

Table 2. Calculated Harmonic Vibrational Frequencies of the Unsubstituted Original Complex **1**

ω (cm^{-1})	symmetry	ω (cm^{-1})	symmetry
138	a_1'		a_1''
192			
253			
309			
338		336	
70	a_2'	103	a_2''
		119	
161		168	
204		197	
63	e'	91	e''
112		146	
143		165	
170		181	
203			
214			
305			
324		321	

We note that the symmetric stretch for the equatorial chloride ligands, pictured in Figure 4, is calculated at 138 cm^{-1} and that for the axial ligands at 338 cm^{-1}. We also observe that the Re−Cl$_{axial}$ bond length is approximately 0.4 Å shorter than the corresponding Re−Cl$_{equatorial}$ bond length. The above-mentioned predicted data clearly show that the Re−Cl$_{equatorial}$ bond is weaker than the Re−Cl$_{axial}$ bond. Therefore, in a ligand substitution dissociative mechanism, where Cl$^-$ is first removed and then H_2O is attached, the preference is clear for the equatorial ligands.

It is difficult to compare our calculated harmonic vibrational frequencies with the experimental data because the former correspond to a single free molecule in the gas phase whereas the latter are either from the crystalline solid state or in a matrix. However, we note two experimental works, the IR analysis by Petrov and Kravchenko[15] and the Raman study by Howard and Andrews.[16] An overall broad agreement of our data with the IR-active e' and a_2'' bands is observed,[15] although the latter do not show the low 63 and 70 cm^{-1} bands, possibly because of inadequacy of the 1971 experiment. Compared to the Raman data,[16] the measured cluster

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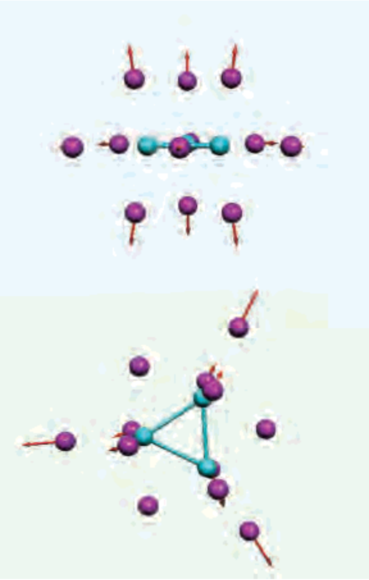

Figure 4. Two a_1' Re−Cl symmetric stretching vibrations of **1**. The bottom is the in-plane 138 cm^{-1} vibration, and the top is the out-of-plane 338 cm^{-1} vibration.

breathing mode at 256 cm^{-1} is calculated by us at 253 cm^{-1}, a really excellent, although possibly to some extent fortuitous, agreement. More generally, it should be commented once again that it is not the purpose of this theoretical work to try to achieve a perfect agreement of calculated geometrical and spectroscopic data with the corresponding experimental because there are too many parameters that differ, with the phase, solvent, and temperature being just a few. We do, however, try to draw, from gas-phase computed data, valid conclusions concerning experiments that refer to solid-state or solution experiments.

2. $[Re_3(\mu\text{-}Cl)_3Cl_8(H_2O)]^{2-}$ (2). The two different structural configurations **2a** and **2b** of the monohydrated complex were fully optimized, and the corresponding minima are shown respectively in Figure 3. It is interesting to note that in both cases the water molecule was left to rotate freely in order to reach a true energy minimum.

Table 1 also summarizes the changes induced on the remaining Re−Cl bonds by introduction of the water molecule. These are, in general, relatively small, except in the case of introduction of an axial water ligand, where a shortening of the order of 0.04 Å occurs for the Re−Re bond opposite to the incoming new ligand.

The conformer **2b** requires some special attention; the minimum-energy structure as shown in Figure 3 corresponds to a shallow local minimum of the potential energy surface, which was at first quite difficult to locate. When disturbed from this shallow minimum, which is confirmed by six “zero” and all positive frequencies, the optimization leads to a structure in which the water molecule is rotated with the H atoms pointing toward the Re cluster, in a position so as to be stabilized by hydrogen bonding with the Cl ligands on the same Re atom. The energy lowering for this structure, which we will name **2b′**, is 0.011 hartree, and the Re−O distance is 3.953 Å, considerably greater than all other computed Re−O distances. For the purpose of comparison of the relative stabilities, we will use structure **2b** and not **2b′** because the former will be dominant in solution (stabilized by hydrogen bonding with neighbors or solvent molecules), where experiments will take place, and hence there will be no need for the water molecule to rotate as in the latter.

Looking at the gas-phase energetics in Tables 1 and 3, we find the cluster **2a** more stable by 14 mhartree or 8.8 kcal/mol, which is reduced to 7.4 kcal/mol when zero-point vibrational corrections are taken into account.

3. $[Re_3(\mu\text{-}Cl)_3Cl_7(H_2O)_2]^{-}$ (3). Six different configurations (structures **3a**−**f**) of the dihydrated complex were considered and fully optimized with respect to the total energy at the DFT/B3LYP level, and the minima obtained are given in Figure 3 and Table 1.

Again, structure **3a** is the one corresponding to the lowest energy, i.e., the most stable in the gas phase. The positioning of the two water molecules is worth some comment; as is clearly seen in the case of **2a**, the axial position is preferred energetically for the water ligands. Hence, one would expect also here the second water ligand to enter in an axial position; electrostatic repulsions and space considerations would have led us to believe that structure **3c** with the two water molecules on different sides of the Re core would have been preferred. However, this structure is found to be 3.38 kcal/mol higher than the most stable **3a**; this can only be attributed to additional stabilization due to hydrogen bonding in the latter.

4. Relative Stability. At first, we will discuss the energy differences between isomeric forms; this in all cases is found to be relatively small. For example, the difference between **2a** and **2b** is 7.4 kcal/mol between zero-point levels. The maximum difference in the case of the dihydrated complex is between **3a** and **3f**, which is 11.23 kcal/mol, but this is an extreme case because two water ligands are forced onto the same Re atom. The difference between **3a** and **3d** is 3.61 kcal/mol between zero-point levels. By comparison, our yet unpublished calculations on the singly reduced $13e^-$ $[Re_3]^{8+}$-cluster, $[Re_3(\mu\text{-}Cl)_3Cl_9]^{4-}$, and the corresponding mono- and dihydrated complexes show these differences to be about 1 order of magnitude larger.

The total (electronic and zero-point) energy difference of a number of conversion reactions is summarized in Table 3.

Conversion from **1** to **2n** is strongly favored energetically, but the energy difference does not appear to be the determining factor of preference between **2a** and **2b**. Conversion from **2n** to **3n′** is also favored, and the calculated energy differences, except for structures **3e** and **3f**, are again not expected to play a very important role in the selection of which product will be dominant.

Finally, we have optimized the trihydrated complex for the case of three equatorial water ligands. This will give us an indication of the energy change for the insertion of a third water molecule in the cluster. As seen in Table 3, the third hydrolysis is found to be endothermic by about 30 kcal/mol and, hence, is not favored energetically.

We have so far reviewed the energetic interpretation from our calculations of the stepwise hydration reactions of **1**.

Table 3. Electronic and Zero-Point Energy Differences of Substitution Reactions

	ΔE_0 (kcal/mol)
1 + H_2O → **2a** + Cl^-	−96.38
1 + H_2O → **2b** + Cl^-	−88.99
2a + H_2O → **3a** + Cl^-	−25.67
2a + H_2O → **3b** + Cl^-	−23.91
2a + H_2O → **3c** + Cl^-	−22.28
2a + H_2O → **3e** + Cl^-	−19.64
2a + H_2O → **3f** + Cl^-	−15.12
2b + H_2O → **3b** + Cl^-	−31.30
2b + H_2O → **3d** + Cl^-	−30.30
2b + H_2O → **3f** + Cl^-	−22.52
3d + H_2O → **4** + Cl^-	+30.51

However, the substitution reaction, and the position selection in each step, will be influenced by two factors: (a) the ease of removal of the outgoing ligand (kinetic factor) and (b) the energetic gain in stability by the incoming ligand (thermodynamic factor).

By looking at the first step, i.e., going from **1** to **2n**, the second factor is present but not considerable because a difference of about 7.4 kcal/mol in the energetic stabilization may easily be overcome by a counteracting kinetic factor. It is therefore reasonable to deduce that if there is a significant kinetic factor, it will determine the selection of the new ligand position. The partial charges, the calculated bond lengths, and the vibrational frequencies all point to the much greater ease of removal of the equatorial chloride ligands and fully agree with the experiment (experimental data are given on p 564 of ref 7, together with their original references).

For the second substitution step, assuming that the first water molecule has entered into an equatorial position, we need to compare structures **3b**, **3d**, and **3f.** Between them, **3b** is of the lowest energy (by 1 kcal/mol compared to **3d** and by 8.78 kcal/mol compared to **3f** and all zero-point-corrected), but again the relatively small energy differences can easily be overcome, allowing the larger kinetic factor to point toward the final product.

The $Re-Cl_{equatorial}$ bond length of the starting complex **2b** is again longer compared to the $Re-Cl_{axial}$ bond length, although this difference is reduced compared to the case of the initial complex **1** (see Table 1). The vibrational frequencies of the in-plane and out-of-plane Re−Cl stretching modes change from 138 and 338 cm^{-1} in **1** to 163 and 350 cm^{-1} in **2b**, respectively. It is therefore clear that the chloride ligand that will be easiest to remove in **2b** will be the second equatorial chloride ligand, thus leading to a kinetic preference for **3d** as the final product.

Hence, the theoretical model predicts that, in a stepwise substitution of the chloride ligands in **1**, both the first and second water molecules will be favored to occupy equatorial positions on two different Re atoms, which is in accordance with the experimental results.

5. Solvent Effects. One of the major problems when using ab initio theoretical methods to treat a reaction that takes place in solution, especially when this reaction involves large clusters of transition metals, is how to take into account the effects of the solvent, counterions, and other agents such as acids, etc. A very good review[17] discusses these issues for the case of water-exchange reactions of metal ions and concludes that the simultaneous use of high-quality DFT methods *and* an exact treatment of the solvent effects is in most cases an impossible task. However, this review concludes that accurate theoretical descriptions of the reactions at a molecular level in the gas phase have confirmed the experimental data.

In our case, the reactions examined take place in solution, with the solvent being water to which a high concentration of HCl is added. Additionally, countercations will be present, which are also found to have in some cases an effect on the solvolysis products. Therefore, as much as it might be desirable to treat this whole system by high-quality DFT, such computations are impossible even with current computing facilities.

Our choice in this work is to perform accurate computations on the isolated main molecules involved in the reactions under examination, in order to provide a solid basic approach to their theoretical understanding. It can be argued that the $[Re_3Cl_{12}]^{3-}$ ion will “see” the solvent environment in an average way, and hence it is the structural properties of each Re−Cl bond that will determine the preference for each hydrolytic step to a greater extent and the average environment to a much lesser extent.

We have examined separately the kinetic and thermodynamic factors of the stepwise hydrolysis of the original isolated anion **1**. To estimate the solvent effect on the $[Re_3Cl_{12}]^{3-}$ anion, we performed a polarized continuum model (PCM)[18] computation and reoptimized the structure including a simulation of the aqueous environment. The $Re-Cl_{equatorial}$ bond length is reduced from 2.734 to 2.671 Å, whereas the $Re-Cl_{axial}$ bond length remains unaffected at 2.346 Å. The symmetric stretching frequencies for the equatorial and axial ligands, which were 138 and 338 cm^{-1}, respectively, are increased to 157 and 346 cm^{-1}, respectively. The conclusions therefore regarding the greater ease of removal of the equatorial ligands are supported in this approximation of the solvent environment. The core is very lightly affected, with the Re−Re bond being shortened in the solvent from 2.469 to 2.457 Å and the $Re-Cl_{bridging}$ bond remaining almost unaffected from 2.463 to 2.461 Å. An attempt to estimate the energy differences (thermodynamic factor) using the PCM model was not made; clearly, the more polar molecules would be favored energetically in the dielectric environment, leading to spurious results because the effects of static hydrogen bonds are not included in the model.

Conclusions

A detailed theoretical study of the stepwise hydrolysis of the $[Re_3(\mu\text{-}Cl)_3Cl_9]^{3-}$ anion has been performed, using very good quality DFT calculations.

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First, we show that, from the energetic point of view, a first and second chloride ligand substitution is possible, but the entry of a third water molecule to the complex will not be favored. Hence, $[Re_3(\mu\text{-}Cl)_3Cl_7(H_2O)_2]^-$ will be a stable product.

As far as the position selection for each step of the hydrolysis, we find the thermodynamic factor to be relatively small and therefore not determining of the result. The kinetic factor, translated as the ease of removal of a chloride ligand, is the factor that both experiment and theory agree on to be decisive of the most preferred conformer produced by the reaction.

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