Theoretical Study of the NaO + HCl Reaction: A Potential Formation Route of NaCl in the Interstellar Medium

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Abstract. A preliminary theoretical characterization of the reaction NaO + HCl in the gas phase and in the presence of a cluster of seventeen water molecules has been carried out. The purpose of this explorative study is to investigate the NaCl + OH reaction for the formation of interstellar NaCl, both in the gas phase and on the surface of amorphous ice of interstellar grains. The reaction was seen to occur without entrance barriers to form an adduct that easily evolves into the NaCl + OH products both in the gas phase and in the presence of the cluster of water molecules. In the case of the cluster reaction, we have simulated an Eley-Rideal mechanism in which HCl approaches, from the gas phase, the NaO radical bound to the 17-water-molecules cluster. Both the gas and ice reactions are strongly exothermic and feasible from a thermodynamic standpoint. Furthermore, being barrierless, they are also expected to be fast under the typical conditions of the interstellar medium. Therefore, this process can be added to the list of reactions to be considered as possible formation routes of the diatomic NaCl molecule in the interstellar medium. More work is needed to better describe this system and other similar reactions, such as those leading to KCl, which is also observed in the interstellar medium.

Keywords: Astrochemistry · Gas Phase · Extraterrestrial Ice · Chlorine · Sodium Chloride · Water-Molecules Cluster

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O. Gervasi et al. (Eds.): ICCSA 2025 Workshops, LNCS 15888, pp. 261–271, 2026.
https://doi.org/10.1007/978-3-031-97596-7_17

1 Introduction

The NaCl molecule has been detected in carbon-rich and oxygen-rich stellar atmospheres [1–7], as well as in the high-mass protostellar disc around Orion Source I [8] and toward the massive proto-binary system IRAS 16547-4247 [9]. In this last study, the authors suggested that molecular lines of NaCl and other alkali halides can play an important role as tracers of the innermost part of the disc, thus allowing the disc to be separated from its envelope. For this reason, it is quite important to understand their formation routes. However, at present, NaCl detection in solar-type star-forming regions and cold clouds remains elusive. The chemistry leading to NaCl has recently been considered in a gas-grain astrochemical model by Acharyya et al. [10], where both gas-phase formation routes and grain chemistry have been considered. All known processes have been reviewed, new ones have been suggested, and the binding energy of several Na-bearing molecules has been estimated [10]. According to that study [10], $NaCl_{(g)}$ can be formed in the gas phase by the radiative association of $Na_{(g)}$ and $Cl_{(g)}$, a process recently characterized by Šimsová et al. [11]. In addition to radiative association, NaCl can be synthesized by a number of reactions between sodium atoms and the Cl-bearing species identified so far in the interstellar medium, including HCl (which is considered one of the main chlorine reservoirs in the interstellar medium [12–14]), or starting from NaH and NaOH [10]. Despite the very large binding energy derived for NaCl on water ice, its formation on the ice surface is considered the dominant process when assuming that 50% of NaCl produced in ice is released in the gas phase by reactive desorption. This suggestion was made in line with the experimental data by Minissale et al. [15] for other diatomic species. Reactions involving sodium monoxide, NaO, have not been considered yet. However, although not detected, NaO is considered a species likely to have astronomical significance due to observational evidence [16] and its presence in several regions of the interstellar medium is indeed plausible since other metal monoxides have been detected (e.g. $FeO_{(g)}$, $AlO_{(g)}$, $TiO_{(g)}$, $CrO_{(g)}$, $VO_{(g)}$, $CaO_{(g)}$ [17–21]). For this reason, we have decided to explore its chemistry with $HCl_{(g)}$ to verify whether NaCl can be readily formed by this process as well. Our choice is also dictated by the fact that sodium atoms might react with water when in contact with numerous water molecules. In fact, some evidence of NaOH formation was obtained when more than one Na atom is adsorbed by a cluster of water molecules or if the water molecules are vibrationally excited ([22,23]).

In this contribution, we present a first explorative study using a density functional theory (DFT) approach to gain a first look at the global potential energy surfaces (PES) of two new possible routes of formation of NaCl, that is, the reaction NaO + HCl in the gas phase:

$$NaO_{(g)} + HCl_{(g)} \rightarrow NaCl_{(g)} + OH_{(g)} \quad (1)$$

and on interstellar amorphous ice simulated by considering a cluster of seventeen water molecules and assuming an Eley-Rideal mechanism in which HCl lands [10] on the NaO radical adsorbed on ice:

$$NaO_{(ice)} + HCl_{(g)} \rightarrow NaCl_{(ice)} + OH_{(ice)} \quad (2)$$

2 Theoretical Methods

The PESs for the two reactions (1) and (2) have been obtained by performing electronic structure calculations at the DFT level of theory. More specifically, all local minima and transition states were optimized using the ωB97XD functional [24], which is known to be suitable for calculating intermolecular interactions such as hydrogen bonds and dispersion forces. For open-shell species, such as NaO, the unrestricted Hartree-Fock (UHF) formalism has been adopted to define the electronic wave function, while the RHF formalism has been used for closed-shell species. The split valence triple zeta polarized basis set 6-311G(d) [25,26], where polarization functions are added for heavy atoms [27], has been used. Calculations were performed using the GAUSSIAN09 program package [28]. The resulting total electronic energies were corrected by adding the zero-point energy (ZPE) and hence obtain enthalpy values at 0 K. Frequency analysis was carried out to assure that the optimized geometries are minima stationary points of the potential energy surfaces. The approach is the same successfully used for other reactions, see Ref. [29–35].

3 Results and Discussion

3.1 The $NaO_{(g)} + HCl_{(g)}$ Reaction

The structures of the reactants and products resulting from our calculations are shown in Fig. 1. The energy and bond lengths compare nicely with the accepted values. For instance, the NaCl and NaO bond lengths are 2.40 and 2.05(6) Å to be compared with the accepted values of 2.36 and 2.05 Å [16,36]. According to our calculations, the gas-phase reaction proceeds with the H-atom transfer from the chlorine atom to the oxygen atom of NaO while, at the same time, a strong interaction between Cl and Na is established. The adduct with the structure reported in Fig. 1(e) is formed via this concerted mechanism in a barrierless process. Notably, even though Na participates in the newly-formed Na-Cl bond, it is still interacting with the oxygen atom that now belongs to the OH group. A small increase of the Na−O bond length can be appreciated (see Fig. 1), while the chemical bond between Na-Cl is almost formed. The adduct is more stable than the reactants by 246.7 kJ/mol at this level of theory. For the isolated system, the large amount of energy released by the adduct formation cannot be dissipated, and the adduct undergoes Na-O bond fission with the formation of the products NaCl + OH. This reactive channel is globally exothermic by 156.9 kJ/mol with respect to the initial NaO + HCl reactants. The calculated reaction

enthalpy at 0 K is in reasonable agreement with the value of -142.6 kJ/mol that can be obtained when using the tabulated enthalpies of formation of reactants and products (see Ref. [37]).

In conclusion, according to our calculations, this barrierless and exothermic reaction is a plausible formation route of interstellar NaCl directly in the gas phase.

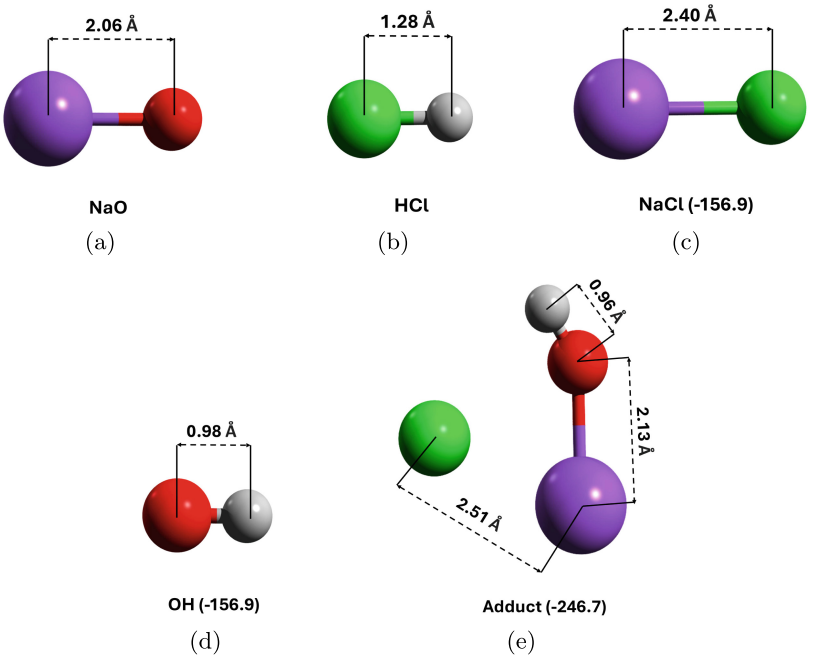
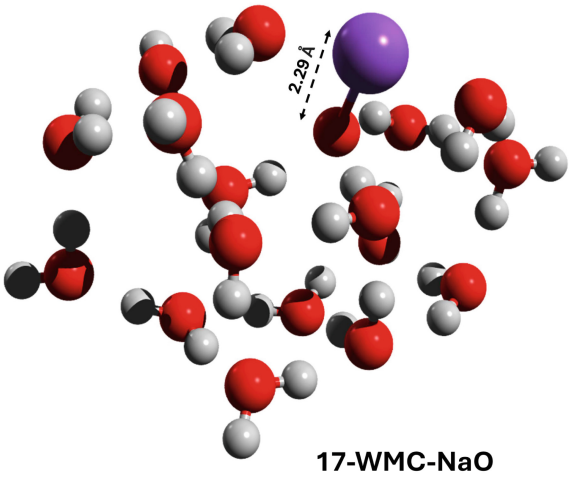


Fig. 1. ωB97XD/6-311G(d) optimized structure and energy (in hartree) of (a) NaO, (b) HCl, (c) NaCl, (d) OH, and (e) the adduct formed in the $NaO_{(g)}$ + $HCl_{(g)}$ reaction. Bond distances in Ångström; energies in parentheses are expressed in kJ/mol with respect to NaO + HCl, regarded as reactants.

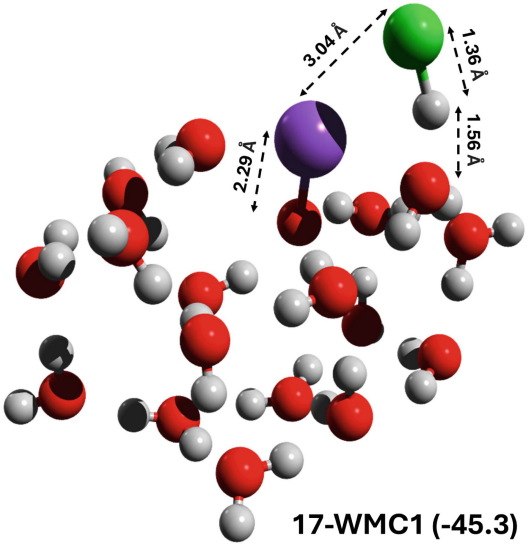
3.2 The NaO + HCl Reaction in a Group of 17 Water Molecules

As anticipated, we have simulated an Eley-Rideal mechanism in which HCl, from the gas phase, interacts with NaO adsorbed on the surface ice, which we simulate with a cluster of water molecules. The 17-water-molecules cluster has been built following a previously derived cluster of 18-water molecules, used to simulate reactions that occur on amorphous ice covering interstellar grains [38–41]. In this work, the number of water molecules in the cluster was due to the replacement of one external water molecule with NaO. Only the most stable NaO adsorption site has been considered here. Its ωB97XD/6-311G(d) optimized

structure (17-WMC-NaO) is shown in Fig. 2(a). Interestingly, the Na−O bond distance, calculated to be 2.29 Å, is larger than the same bond distance for the isolated molecule depicted in Fig. 1(a). This is in line with what is expected because of the increased ionic character of the NaO bond in the presence of the polar water molecules of the cluster. Indeed, as indicated by the Mulliken partial atomic charges with respect to those of the isolated NaO, a slightly higher ionic degree of the sodium/oxygen pair (−0.621/0.630 e) is computed. The optimized structure of NaCl embedded in the 17-water-molecules cluster (17-WMC-NaCl) is shown in Fig. 2(d). We have determined this structure as a reference point to establish if the interaction between $HCl_{(g)}$ and $NaO_{(ice)}$ produces the expected NaCl product. Also in this case, the bond distance between sodium and chlorine, calculated to be 2.65 Å, is larger than the same atomic distance of the isolated molecule depicted in Fig. 1(a) and an examination of the Mulliken charge distribution reveals a larger charge separation (-0.854/0.666 e) with respect to the isolated NaCl (−0.652/0.652 e). When considering the interaction of $HCl_{(g)}$ with $NaO_{(ice)}$, our calculations identified two stationary points that unveil the ongoing reaction mechanism. A first intermediate (17-WMC1, see Fig. 2(b)) is formed, more stable than the reactants by 45.3 kJ/mol. The approaching HCl molecule has oriented itself in such a way that chlorine interacts with the Na atom of NaO, while the H atom interacts with a lone pair of a water molecule. This first intermediate can easily evolve (without an energy barrier) into another structure (17-WMC2, see Fig. 2(c)) that can be taken as the ending point of the reaction. Indeed, the NaCl bond distance (2.60 Å) has a value comparable to that of the optimized structure of NaCl in the water cluster (2.65 Å). Nevertheless, the sodium atom is still considerably interacting with the O atom (the bond distance has only increased from 2.29 to 2.31 Å) while the H−Cl bond length has significantly increased (from 1.28 Å of the isolated gas-phase molecule to 1.36 Å in 17-WMC1 up to 1.85 Å in the product-like final structure 17-WMC2). The global energy gain with respect to the reactants is 71.2 kJ/mol, making this mechanism exothermic. We did not explore that further, but it is probable that a proton relay process occurs at this stage, eventually leading to the OH coproduct. It is interesting to note that, while in many other cases the presence of water molecules [31,38–44] stabilizes the reaction intermediates with respect to the reactants, here the opposite is true. This simply means that the stabilizing effect of the cluster of seventeen water molecules is smaller for the intermediate and the products than for $NaO_{(ice)}$. However, the overall reaction remains exothermic and the reactants are easily converted into NaCl. The hydrogen bonds provide a stabilizing effect: when the NaO radical is considered on the water cluster, the binding energy is on the order of hundreds kJ/mol (ca. 250 kJ/mol). Notably, Eley-Rideal mechanisms (that is, processes in which one of the reactants is adsorbed on the ice surface with the other coming from the gas phase) are considered important mechanisms in interstellar regions characterized by high atomic densities [45,46].

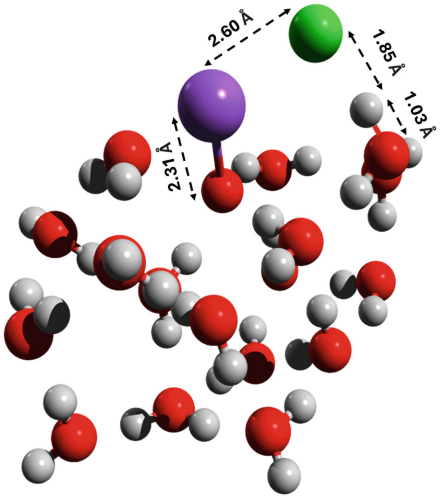


(a)



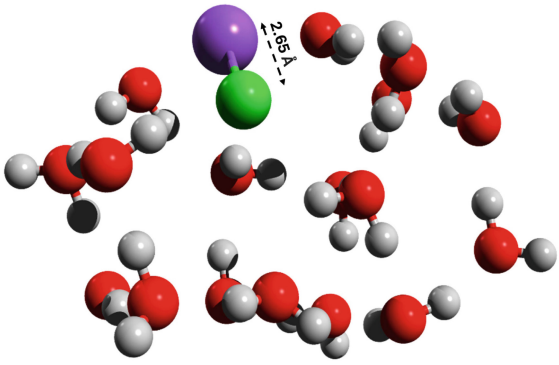
(b)

Fig. 2. ωB97XD/6-311G(d) optimized structure and energy of (a) NaO adsorbed in the 17-water-molecules cluster (the most stable arrangement); (b) the intermediate arising from the reaction between NaO adsorbed in the 17-water-molecules cluster with HCl from the gas phase; (c) the post-reaction structure arising from the establishment of the Na−Cl bond and H-transfer from the Cl atom to one of the O atoms of the 17-water-molecules cluster; (d) the optimized structure of NaCl adsorbed on the 17-water-molecules cluster. Bond distances in Ångström; energies in parentheses are expressed in kJ/mol with respect to the 17-WMC-NaO $+HCl_{(g)}$.



17-WMC2 (-71.2)

(c)



17-WMC-NaCl

(d)

Fig. 2. (*continued*)

4 Conclusion and Implications in Astrochemistry

In this work, the reaction between NaO and HCl has been investigated considering the two possible media where reactions can occur in interstellar environments, that is, the gas phase and the icy mantles of interstellar grains. Grain chemistry has been simulated by considering a cluster of seventeen water molecules as a model for amorphous ice and an Elay-Rideal mechanism in which HCl comes from the gas phase. The presence of the water molecules does not significantly

alter the reaction mechanism. In both cases, the reactions are barrierless and evolve through intermediates located well below the energy asymptote of the reactants. We have planned further calculations to better describe these systems at a higher level of theory to confirm the results of this preliminary investigation.

Concerning the possible implications in astrochemistry, our study indicates that the gas-phase $NaO_{(g)} + HCl_{(g)}$ reaction is another possible formation route of NaCl directly in the gas phase where it has been observed. We have not derived the rate coefficient, but being barrierless in the entrance channel and very exothermic, reaction (1) is expected to have a rate coefficient in the gas-kinetics limit, that is, around 10^{-10} cm^3 s^{-1}. Therefore, it is as efficient as the other gas-phase reactions considered in the model by Acharyya et al. [10], that is, $NaOH_{(g)} + HCl_{(g)}$, $NaH_{(g)} + Cl_{(g)}$, and $Na_{(g)} + HCl_{(g)}$. The importance of these reactions, therefore, depends on the abundance of the reactants. $NaOH_{(g)}$ and $NaH_{(g)}$, as well as $NaO_{(g)}$, have not yet been detected, and therefore it is difficult to judge their relative importance.

As regards the reactions on ice, according to the model by Acharyya et al. [10], the dominant processes are $Na_{(ice)} + Cl_{(ice)} \rightarrow NaCl_{(ice)}$ and $NaH_{(ice)} + Cl_{(ice)} \rightarrow NaCl_{(ice)} + H_{(ice)}$. The $Na_{(ice)} + Cl_{(ice)}$ reaction is dominant up to 10^5 years. Hydrogenation of $Na_{(ice)}$ and $Cl_{(ice)}$ are competing processes that could suppress the importance of $Na_{(ice)} + Cl_{(ice)} \rightarrow NaCl_{(ice)}$. Furthermore, Na can react with water in large water clusters or in the presence of more than one Na atom [22,23]. Furthermore, in the astrochemical model by [10], this specific formation route of NaCl in ice is so important because it is assumed that 50% of it is released in the gas phase by reactive desorption. This suggestion was made upon the indications of the experimental work by Minissale et al. [15] for other diatomic species that, however, are very different with respect to NaCl (e.g., O2, N2). Indeed, their conclusion was that chemical desorption is a favorable process for diatomic molecules with low binding energies formed by recombination reactions. This is also confirmed by ab initio molecular dynamics simulations of H_2 formation on periodic crystalline and amorphous ice surface models ([47]). However, NaCl is characterized by a very large binding energy of 14000 K [10] and, therefore, it is quite different compared to the cases analyzed by Minissale et al. [15]

The characterization of NaCl formation pathways in the interstellar medium is still in its infancy. More theoretical and experimental data are needed.

Acknowledgments. GDG, NB, CC, and PU thank the MUR PRIN2020 (2020AFB3FX-Astrochemistry beyond the second-period elements) and the European Union's Horizon 2020 research and innovation program from the European Research Council (ERC) project 'The Dawn of Organic Chemistry' (DOC), grant agreement no 741002) for support. AG and MR thank financial support under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 104 published on 2.2.2022 by the Italian Ministry of University and Research (MUR), funded by the European Union - NextGenerationEU - Project Title 2022JC2Y93 ChemicalOrigins: linking the fossil composition of the Solar System with the chemistry of protoplanetary disks - CUP J53D23001600006 - Grant Assignment Decree No. 962 adopted on 30/06/2023 by the Italian Ministry of University and

Research (MUR). NB and PU acknowledge support from the Italian Space Agency (Bando ASI Prot. n. DC-DSR-UVS-2022-231, Grant no. 2023-10-U.0 MIGLIORA). AR thanks the European Union's Horizon 2020 research and innovation program from the European Research Council (ERC) for the project 'Quantum Chemistry on Interstellar Grains' (QUANTUMGRAIN), grant agreement no. 865657. PU acknowledges support from the Project CH4.0 under the MUR program "Dipartimenti di Eccellenza 2023-2027" (CUP: D13C22003520001).

Disclosure of Interests. None of the authors have any conflicts of interest to declare.

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