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Dynamic Investigations of Rare Gas-NO+ Interactions

Fatih ÖZKALAYCI[1*]

ABSTRACT: In this work, integral cross sections and rate constants of ground states of the Rg-NO$^+$ (X1Σ+) system were calculated from quantum mechanical approach. The Rg separately defines the three inert gaseous of He, Ne and Ar elements. Equilibrium geometry values of the Rg-NO$^+$ (X1Σ+) complexes were calculated employing the CCSD(T)-F12 method with cc-pVTZ-F12 basis set augmented with mid-bond functions. After using analytical forms of the potentials, vibrational frequencies and dissociation energies were calculated. The dissociation energy values of 196.6, 364.4 and 1045.0 cm^{-1} were found for He-NO$^+$, Ne-NO$^+$ and Ar-NO$^+$ systems, respectively. Zero-point energy (ZPE) values of the systems were found to be 1240.4, 1251.6 and 1284.9 cm^{-1} for He-NO$^+$, Ne-NO$^+$ and Ar-NO$^+$ systems, respectively. Differential cross sections and rate constants were found in a broad range of energy and temperature for He, Ne and Ar rare gaseous. The rank order of the magnitudes of the rotational transition rate coefficients was compared and it was found that they can differ slightly for a few temperatures. Integral cross sections and collision rate constants were compared to those of experimental and theoretical studies in literature and they were found to be well agreed.

Keywords: *Ab initio* calculations, diatomic interactions, integral cross sections, rate constants

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INTRODUCTION

Rg-NO$^+$ systems were studied in this work in order to understand interaction mechanisms of the He, Ne and Ar with NO$^+$. Understanding of particle interactions with molecules is crucial for both interstellar medium (ISM) and Earth's atmosphere from the point of astrophysics. Formation of weakly bound molecular complexes is undoubtedly an important phenomenon playing a crucial role for atmospheric reactions, astrophysics and biochemistry. Due to being one of the most stable diatomic ions and most abundant species in the upper atmosphere (Albritton et al., 1979), NO$^+$ has key importance for astrophysical aspect. The possible existence of NO$^+$ and most probable mechanisms of formation of NO$^+$ in the interstellar medium were first discussed in 1970's (Herbst and Klemperer, 1973; Pickles and Williams, 1977; Singh and Maciel, 1980) and the NO$^+$ was discovered by Cernicharo et al. in 2014 (Cernicharo *et al.*, 2014). This first detection of NO$^+$ in the cold dense core of Barnard 1-b was an important step in understanding the interstellar chemistry of molecules containing N and O atoms. Due to these interests of NO$^+$ cation, NO$^+$ has been widely studied. Both theoretical and experimental studies studied equilibrium geometries, vibrational frequencies and ionization energies of mostly Ar-NO$^+$ (Takahashi, 1992; Fourré and Raoult, 1995; Wright, 1996; Bush *et al.*, 1997; Halvick *et al.*, 2011) but Rg-NO$^+$ (Lee et al., 1998; Lee et al., 2000; Soldan et al., 2002; Adler et al., 2007; Knizia et al., 2009) complexes.

On theoretical side, Soldan et al. (Soldan et al., 2002) and Robbe et al. (Robbe et al., 1993) studied He-NO$^+$ complex Wright and coworkers (Wright et al., 1994; Bush *et al.*, 1997; Lee et al., 1998) studied Ar-NO$^+$ using different *ab initio* methods. Robbe et al. (Robbe et al., 1993) determined bent structure for NO$^+$ cation. Fourre and Raoult (Fourré and Raoult, 1995) studied vibrational structure of Ar-NO$^+$ complex. Halvick et al. (Halvick *et al.*, 2011) constructed a new potential energy surface for Ar-NO$^+$ complex with CCSD(T)-F12 method. Interactions between rare gaseous including Kr and Xe and NO$^+$ were studied by Lee et al. employing different *ab initio* methods from 2nd order Moller-Plesset to coupled cluster approaches. Sato et al. (Sato et al., 1984) and Takahashi (Takahashi, 1992) exprementally studied Ar-NO$^+$ cation.

In this study, Rg-NO$^+$ system studied for He, Ne and Ar gaseous using correlated coupled cluster method including single, double and non-iterative triple excitations (CCSD(T)-F12) (Adler et al., 2007; Knizia et al., 2009) with correlation-consistent, triple-zeta (cc-pVTZ-F12) basis sets augmented with additional mid-bond functions. Harmonic and anharmonic vibrational frequencies of the complexes were calculated. Integral cross sections and rate constants were calculated and they were compared with the literature. This paper is organized as follows: a discussion on the methods is presented in Section 2. Results are discussed in Section 3. Rate coefficients and cross sections are given in Section 4 and conclusions are presented in Section 5.

MATERIALS AND METHODS

Jacobi coordinate system, which is shown in Figure 1, was used in this work. Origin of the coordinate system is the center of mass of the NO$^+$ molecule, and R defines the distance between Rg atom and centre of mass of NO$^+$ molecule. θ shows the angle between the directions of NO$^+$ molecule and origion-Rg molecule, and angle starts to rise from N side of the molecule. Equilibrium distance of NO$^+$ was kept fixed at 2.0125 a_0 during the calculations while experimental equilibrium distance of NO$^+$ molecule was found as 2.0124 a_0 (Irikura, 2007) which agrees perfectly with our result of 2.0125 a_0. All the calculations are done under conditions of that the diatomic NO$^+$ molecule were kept rigid at its equilibrium value of 2.0125 a_0. MOLSCAT (MOLecular SCATtering), which is a time-independent quantum method based on Fortran programming code, was used for dynamic properties of the systems.

Like all time-independent programs, Molscat gives better results on getting quantum mechanical data especially for low collision energies. Molscat code for quantum mechanical solution of the nonreactive molecular scattering problem was developed to obtain collision rates for molecules in the interstellar gas which are needed to understand microwave and infrared astronomical observations (Hutson and Green, 2012).

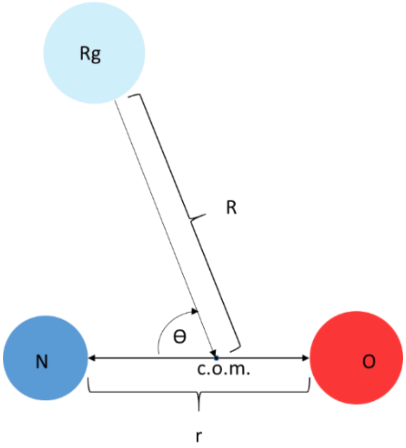

Figure 1. Jacobi coordinate of the Rg-NO$^+$ complex system

1∑+ describes the ground state electronic levels of the NO$^+$ cation. Basis set was augmented with a set of bond functions at mid-distance between the Rg and the NO$^+$ center of mass in order to improve dispersion component of the interaction. Explicitly correlated coupled-cluster methods that include single, double, and non-iterative tirple excitations (CCSD(T)-F12) (Adler et al., 2007; Knizia et al., 2009) and cc-pVTZ-F12 basis set were used in calculations. MOLPRO *ab initio* program (Werner *et al.*, 2012) was used to analyse the interaction mechanisms.

Preliminary, equilibrium geometries of the Rg-NO$^+$ complexes are optimized. All internuclear distances were optimized. Harmonic and anharmonic vibrational frequencies of the complexes were calculated for stretching and intermolecular bending of the complex and NO$^+$ intramolecular stretch. Geometric parameters are listed in Table 1. Calculations of the interaction energies were carried then out for 47 intermolecular distances from 3.5 to 100 a_0, while the angular grid for the θ variable consisted of 19 values for every 10º from 0 to 180º for every 10º angle. Electronic structure calculations results are done for a discrete set of the total 6384 points in Jacobi (R, θ) coordinate system. In all the calculations, the internuclear NO$^+$ distance was frozen at the equilibrium distance (2.0125 a_0). The basis set superposition errors (BSSE) in all geometries were corrected by the standard counterpoise correction scheme of Boys and Bernardi (Boys and Bernardi, 1970) to determine the interaction potential defined as:

$$E_I(R,\theta) = E_{Rg-NO^+}(R,\theta) - E_{NO^+}(R,\theta) - E_{Rg}(R,\theta) \quad (1)$$

Integral Cross Sections

Total cross sections of the systems were obtained with the Molscat program by using the obtained scattering matrix. Since the Rg-NO$^+$ interaction did not result in a reaction, only the inelastic behavior of the target molecule was investigated due to the vibrational and rotational levels of the target molecule was excited depending on the collision energy. The integral cross section $\sigma_j(E_k)$, which is a function of the collision energy for the initial rotational state j of the molecule, is given by the sum over all values of the total angular momentum quantum number of the reaction probabilities. Inelastic integral cross sections from initial rotational state j to final state j' of product molecule is given as (Arthurs and Dalgarno, 1960):

$$\sigma_{j\to j'}(E_k) = \frac{\pi}{(2j+1)k_j^2} \sum_{J=0}^{\infty} (2j+1) \sum_{l=|J-j|}^{|J+j|} \sum_{l'=|J-j'|}^{|J+j'|} \left| \delta_{jj'}\delta_{ll'} - S^{J}_{j'l';jl}(E) \right|^2 \qquad (2)$$

where J, l and E are total angular momentum quantum number, orbital angular momentum quantum number and the total energy, respectively. Energy is given as follows:

$$E_k = \frac{\hbar^2 k_j^2}{2\mu} = E - \varepsilon_j \qquad (3)$$

where ε_j and μ are energy of initial rotational energy state of j and reduced mass, respectively.

Rate Constants

State-to-state rate constants for this reaction have been calculated from quantum calculations.

Thermal rate constant for an interaction of $X + YZ \to XY + Z$ is given as follow (Hirst, 1985):

$$-\frac{d[n_X]}{dt} = -\frac{d[n_{YZ}]}{dt} = k(T)[n_X][n_{YZ}] \qquad (4)$$

If the quantum mechanical states are considered in a reaction like $X + YZ(\nu, j) \to XY(\nu', j') + Z$, rate constant can be written as:

$$-\frac{d[n_X]}{dt} = -\frac{d[n_{YZ}(\nu,j)]}{dt} = \sum_{\nu'j'} k_{\nu j,\nu'j'}(T)[n_X][n_{YZ}(\nu,j)] = k_{\nu j}(T)[n_X][n_{YZ}(\nu,j)] \qquad (5)$$

where $k_{\nu j}(T)$ is the reaction rate constant for the ν and j quantum states.

The thermal rate constant is obtained by integrating the total cross sections over all energies (or velocity vectors) according to the Maxwell-Boltzman distribution and it is given:

$$k(T) = \int E\sigma(E)f(E,T)dE \qquad (6)$$

where $f(E,T)$ is Maxwell-Boltzmann distribution function. By taking the Boltzmann thermal average of the cross sections from the rotational excitation cross section $\sigma_{j\to j'}(E_k)$, the rotational excitation rate constant at temperature T is given as follows:

$$k_{j\to j'}(T) = \left(\frac{8k_BT}{\pi\mu}\right)^{\frac{1}{2}} \frac{1}{(k_BT)^2} \int_0^{\infty} \sigma_{j\to j'}(E_k) \exp\left(-\frac{E_k}{k_BT}\right) E_k dE_k \qquad (7)$$

where k_B and E_k are Boltzmann constant and collision energy, respectively (Denis-Alpizar and Stoecklin, 2015).

RESULTS AND DISCUSSION

He-NO$^+$ complex was studied by Soldan et al. (Soldan et al., 2002) and Robbe et al. (Robbe et al., 1993). Ar-NO$^+$ was studied by Wright and coworkers (Wright et al., 1994; Wright, 1996; Bush *et al.*, 1997) by using different *ab initio* methods. Robbe et al. (Robbe et al., 1993) determined bent structure for NO$^+$ cation. Vibrational structure of Ar-NO$^+$ complex was carried out by Fourre and Raoult (Fourré and Raoult, 1995). Halvick et al. (Halvick *et al.*, 2011) constructed a new potential energy surface for Ar-NO$^+$ complex. Interactions between rare gaseous including Kr and Xe and NO$^+$ were studied by Lee et al. (Lee et al., 1998) employing different *ab initio* methods from 2nd order Moller-Plesset to coupled cluster approaches. Also, Sato et al. (Sato et al., 1984) and Takahashi (Takahashi, 1992) exprementally studied Ar-NO$^+$ cation.

Electronic structure calculations results are done for a discrete set of the total 6,384 points in Jacobi (R, θ) coordinate system sketched in Figure 1. Furthermore, molecular geometry parameters and some frequency values were given in Table 1. Equilibrium bond distance values of NO$^+$ are found 2.013 a_0 for He-NO$^+$ and Ne-NO$^+$ complexes and 2.014 a_0 for Ar-NO$^+$ complex. Equilibrium bond distances of He-NO$^+$, Ne-NO$^+$ and Ar-NO$^+$ are found to be 5.25, 5.37 and 5.87 a_0, respectively. Stoecklin et al. (Stoecklin and Voronin, 2011) found the well depth and interaction angle of the He-NO$^+$ complex as 195.4 cm^{-1} and 80.4°, respectively. Halvick et al. (Halvick *et al.*, 2011) found the equilibrium geometry values of the Ar-NO$^+$ system as r=re=2.01 a_0, R=5.86 a_0, and θ= 66.8° from the three-dimensional potential energy surface, which are close to those found by Wright et al. (Wright et al., 1994). The ground state dissociation energy, equilibrium distances of re, R and angle of θ for the Ar-NO$^+$ system was found as 951.0 cm^{-1}, 2.14 a_0, 5.87 a_0 and 66.7° in this study, respectively. Equilibrium bond distance values of Rg-NO$^+$ and NO$^+$ are well agreed with those in literature (Wright, 1996; Lee et al., 1998; Soldan et al., 2002; Orek *et al.*, 2016). Frequencies of bending (ϖ1), strectching (ϖ2) ve intermolecular stretching for NO$^+$ (ϖ3) are found as 107.8, 81.5 and 119.1 cm^{-1} for He-NO$^+$, Ne-NO$^+$ and Ar-NO$^+$ complexes, respectively. These values agree well with those of 107, 82 and 111 cm^{-1} found by Lee et al. (Lee et al., 1998) for He, Ne and Ar containing complex systems, respectively. Dissociation energies and zero-point energies of the complexes were also shown in Table 2. The dissociation energy values of 196.6, 364.4 and 1045.0 cm^{-1} were found for He-NO$^+$, Ne-NO$^+$ and Ar-NO$^+$ systems, respectively. Zero-point energy (ZPE) values of the systems were found to be 1240.4, 1251.6 and 1284.9 cm^{-1} for He-NO$^+$, Ne-NO$^+$ and Ar- NO$^+$ systems, respectively. Dissociation energy and zero-point energy values are agreed with the literature (Takahashi, 1992; Si-sheng *et al.*, 2007; Halvick *et al.*, 2011).

Table 1. Equilibrium parameters of Rg-NO$^+$ complexes. Bending (ϖ1), strectching (ϖ2) ve intermolecular stretching for NO$^+$ (ϖ3) frequencies

Sistem	**Referans**	***r$_e$(NO$^+$)*(Å)**	**R$_e$ (Å)**	**Θ (°)**	**ϖ$_1$(eV)**	**ϖ$_2$ (eV)**	**ϖ$_3$ (eV)**
He-NO$^+$	This work	1.065	2.777	79.71	0.005	0.013	0.294
	(Orek et al., 2016)	1.065	2.793	80.2	0.005	0.014	0.294
	(Soldan et al., 2002)	1.063	2.788	79.3	-	-	-
	(Lee et al., 1998)	1.063	2.788	84.3	0.004	0.013	0.300
Ne-NO$^+$	This work	1.065	2.841	76.78	0.006	0.010	0.294
	(Orek et al., 2016)	1.065	2.793	80.02	0.006	0.010	0.030
	(Lee et al., 1998)	1.082	2.793	91.3	0.005	0.010	0.267
	(Lee et al., 1998)	1.063	2.809	90.8	-	-	-
Ar-NO$^+$	This work	1.065	3.105	66.74	0.011	0.015	0.293
	(Orek et al., 2016)	1.066	3.068	70	0.011	0.015	0.293
	(Lee et al., 1998), (Wright, 1996)	1.065	2.989	75.9	0.010	0.014	0.298
	(Halvick et al., 2011)	1.065	3.100	66.2	0.011	0.015	0.293
	(Takahashi, 1992)	-	-	-	0.010	0.012	-

Table 2. Zero-point energy and dissociation energy values of complexes

Sistem	**ZPE (eV)**	**De (eV)**	**D0 (BOUND) (eV)**
He-NO+	0.1538	0.0244	0.0163
Ne-NO+	0.1552	0.0452	0.0377
Ar-NO+	0.1593	0.1296	0.1179
NO+	0.1472		

For the calculation of dynamic quantities such as collision cross sections and rate constants, the potential energy surfaces obtained by *ab initio* methods were used in the time-independent Schrödinger equation, and collision cross sections and rate constants for Rg-NO$^+$ systems were calculated by solving the time-independent Schrödinger equation and using Equation 2 and Equation 7, respectively. The close coupling inelastic cross sections of the complex systems were computed for collisional energy varying from 10^{-5} to 1000 cm^{-1}. Integral cross sections as a function of collision energy graphs were given in Figures 2, 3 and 4 for He- NO$^+$, Ne- NO$^+$ and Ar- NO$^+$, respectively.

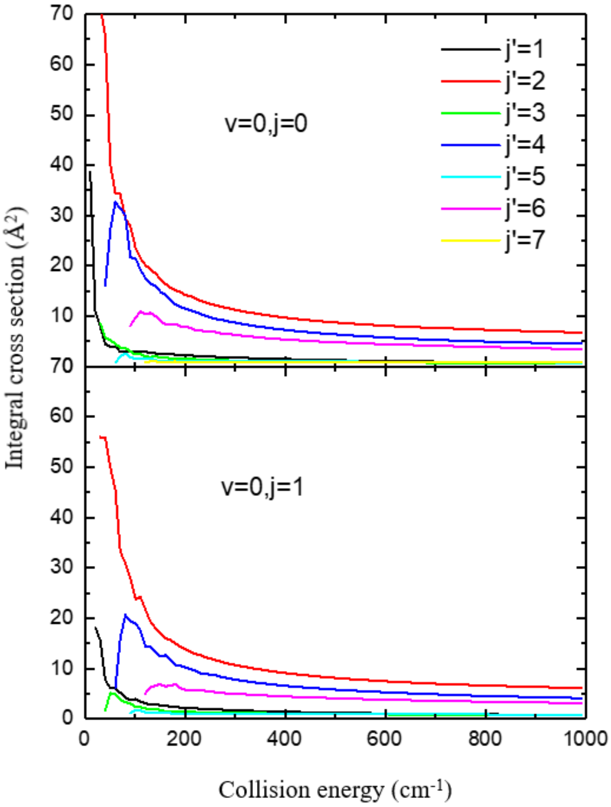

Figure 2. Depiction of integral cross sections in Å^2 for He+NO$^+$(v=0, j=0,1)→He+NO$^+$(j') for j'=0-7 as a function of the collision energy in cm^{-1}

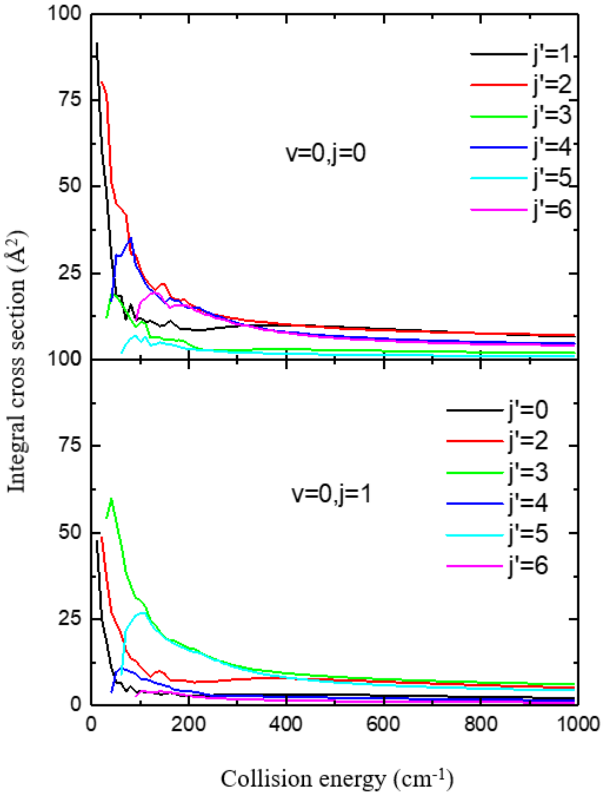

Figure 3. Depiction of integral cross sections in Å^2 for Ne+NO$^+$(v=0, j=0,1)→Ne+NO$^+$(j') for j'=0-7 as a function of the collision energy in cm^{-1}

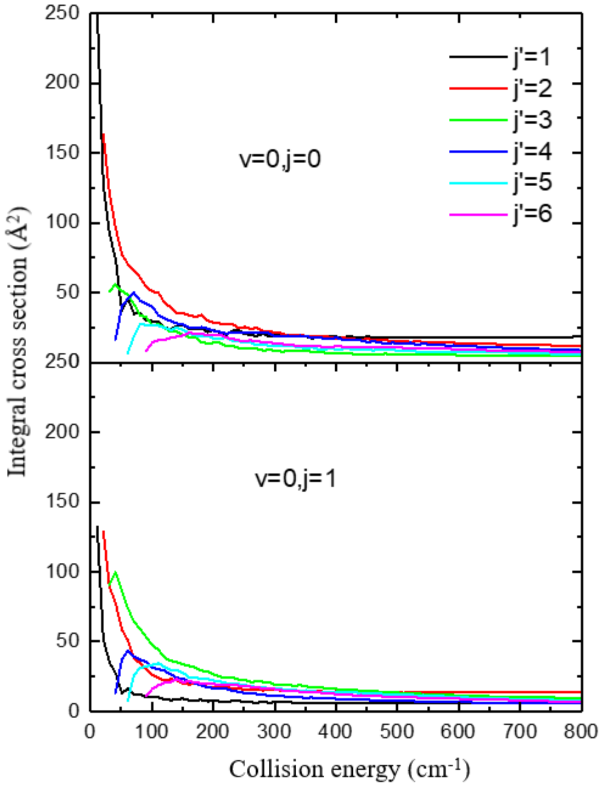

Figure 4. Depiction of integral cross sections in Å^2 for Ar+NO$^+$(v=0, j=0,1)→Ar+NO$^+$(j') for j'=0-7 as a function of the collision energy in cm^{-1}

Integral cross sections were given for He-NO$^+$ interaction for vibrational and rotational energy levels in Figure 2. This interaction mechanism was examined for v=0 vibration and j=0,1 rotation energy levels. Integral cross section values were found to be higher at lower collision energies, and they decreased exponentially with increasing collision energy for both v=0 and j=0,1 energy levels. Morever, integral cross sections were found constant trend at energies higher than 600 cm^{-1}. Integral cross sections for energy levels of v=0,j=0 were also found to be higher than those of v=0,j=1. It was obvious from Figure 2 that integral cross sections obtained for even-rotation quantum states of the product molecule are larger than for odd-numbered quantum states.

In Figure 3 Integral cross sections were sketched for Ne-NO$^+$ interaction mechanism for v=0 and j=0,1 vibrational and rotational energy levels. Integral cross section values were found to be higher at lower collision energies, and they decreased exponentially with increasing collision energy for both v=0 and j=0,1 energy levels as in He-NO$^+$ interaction mechanism. At energies higher than 600 cm^{-1}, integral cross sections were found almost constant. Integral cross section values for energy levels of v=0,j=0 were also found to be higher than those of v=0,j=1. It was also obvious from Figure 3 that integral cross sections obtained for even-rotation quantum states of the product molecule are larger than for odd-numbered quantum states. It can also be easily seen that the integral cross sections obtained for Ne are larger than the those obtained for He from Figure 2 and Figure 3. The main reason for this can be said that the Ne atom has more mass than the He atom, as well as the higher rotational quantum numbers and the potential energy surface obtained for Ne is much more effective in dynamical calculations.

Integral cross sections were given for Ar-NO$^+$ interaction mechanism for v=0 and j=0,1 vibrational and rotational energy levels in Figure 4. Integral cross section values were higher at lower collision energies, and they decreased exponentially with increasing energy for both v=0 and j=0,1 energy levels as in previous interaction mechanisms. Integral cross section values showd constant trend at higher energies than 600 cm^{-1} as in He-NO$^+$ and Ne-NO$^+$ systems. Integral cross section values for energy levels of v=0,j=0 were also found to be higher than those of v=0,j=1. It was also obvious from Figure 3 that integral cross sections obtained for even-rotation quantum states of the product molecule are larger than for odd-numbered quantum states. It can also be easily seen that the integral cross sections obtained for Ne are larger than the those obtained for He from Figure 2 and Figure 3. Integral cross sections obtained for the Ar system are larger than those obtained for Ne and He systems. This situation is expected to show itself in rate constants as well.

By using the integral cross section values, rotational rate coefficients were calculated for the same quantum states by using Equation 7. Figure 5 depicts the dependence of the rotational rate coefficients as a function of the temperature for transitions from j=5 rotational level for the ground vibrational state of NO$^+$ for He-NO$^+$ complex system. The same representation is given in Figures 6 and 7 for Ne-NO$^+$ and Ar-NO$^+$ complexes, respectively. Rate constants of all the systems were calculated for v=0,j=5 quantum states due to fact that 5 is the highest rotational quantum state number. The rate coefficients associated with the rotational transitions from ν = 0 and j=5 levels to the ν = 0 and j = 0, 1, 2, 3 and 4 final rotational levels for the of NO$^+$ at selected temperatures. Differences in magnitudes between rotational rate coefficients for He and Ne molecules are less than 10^{-1} for $j>0$ but less than 10^{-2} for j=0. Similar propensity was also found for Ar-NO$^+$ complex but slightly higher than both He-NO$^+$ and Ne-NO$^+$ complexes for each rotational energy level. Dependence on temperature for an initial quantum number j_i are seen to get higher for lower temperatures and then rate coeffiecient values vary very slowly with increasing temperature. Though the differences are small, it is also important to notice that the rotational transition rate coeffients is a function of temperature and there are differences for each rare gas. He-NO$^+$ interaction mechanism results agree well with a study [30] carried out Stoecklin et al. Rate constant values get higher a little at low temperatures and showed a onstant trend with increasing temperature.

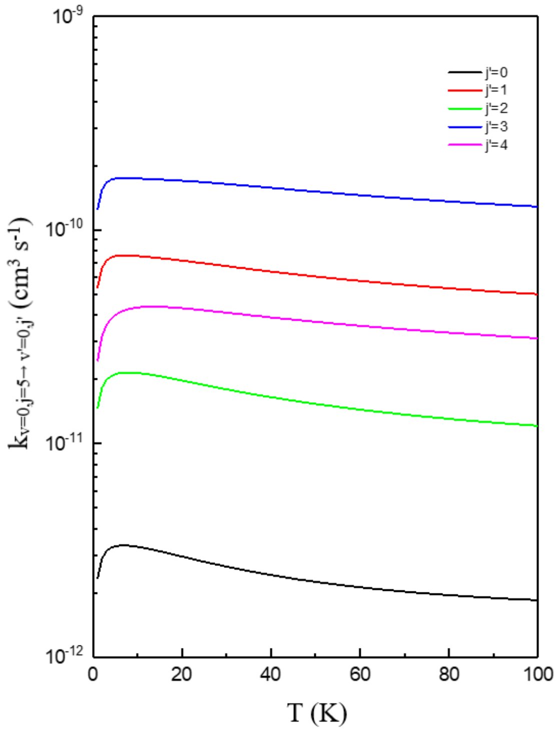

Figure 5. Rotational rate coefficients of NO$^+$ (ν = 0, j = 5→ ν =0, j') for j'=0-4 in collision with He as a function of temperature

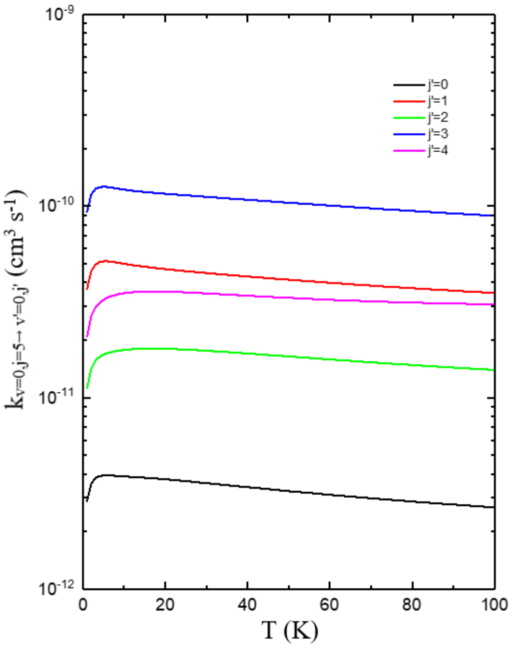

Figure 6. Rotational rate coefficients of NO$^+$ ($v = 0, j = 5 \rightarrow v = 0, j'$) for j'=0-4 in collision with Ne as a function of temperature

Rate constants obtained for the interaction of the Ne atom with the NO$^+$(v=0,j=5) molecule are shown in Figure 6 as a function of temperature for the rotational quantum states of the product molecule. Here again, rate constants were found larger for odd quantum numbers of product molecule due to the odd parity behavior. In Figure 7, rate contants of Ar-NO$^+$(v=0,j=5) Ar-NO$^+$(v'=0,j') interaction mechanism were given as a function of temperature. The rate constants of Ar-NO$^+$ complex system were found the higgest compared to other He-NO$^+$ and Ne-NO$^+$ complex systems. This situation was also observed for integral cross sections for each interaction mechanisms. Rate constants which is expressing the events per cm^3 in one second are not affected by high temperatures.

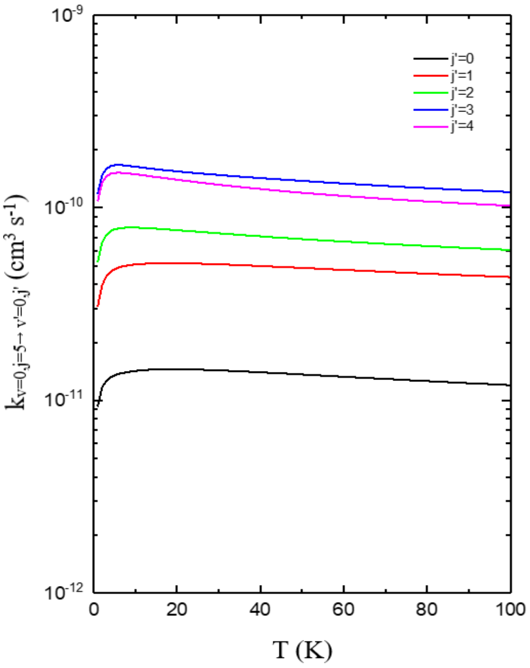

Figure 7. Rotational rate coefficients of NO$^+$ ($v = 0, j = 5 \rightarrow v = 0, j'$) for j'=0-4 in collision with Ar as a function of temperature

CONCLUSION

Dynamic properties of Rg-NO^+ (X1Σ+) van der Waals systems were computed using the calculated with explicitly correlated CCSD(T)-F12 method with cc-pVTZ-F12 basis set with midbond functions basis set. CCSD(T)-F12/cc-pVTZ-F12 level of theory which is an accurate approach for the generation of highly correlated potential energy surfaces was used. Integral cross sections and rate coefficients of He-NO^+, Ne-NO^+ and Ar-NO^+ systems are discussed. Equilibrium bond distance values of NO^+ are found 2.013 a_0 for He-NO^+ and Ne-NO^+ complexes and 2.014 a_0 for Ar-NO^+ complex. Equilibrium bond distances of 5.25, 5.37 and 5.87 a_0 are found for He-NO^+, Ne-NO^+ and Ar-NO^+, respectively. The dissociation energy values for He-NO^+, Ne-NO^+ and Ar-NO^+ systems were found 196.6, 364.4 and 1045.0 cm^{-1}, respectively. Zero-point energy (ZPE) values of the systems were 1240.4, 1251.6 and 1284.9 cm^{-1} for He-NO^+, Ne-NO^+ and Ar- NO^+ systems, respectively. Integral cross section values were found to be higher at lower collision energies, and they decreased exponentially with increasing collision energy for both v=0 and j=0,1 energy levels. The rate constants of Ar-NO^+ complex system were found larger than those of the other two systems of He-NO^+ and Ne-NO^+. There is good agreement found between the results and the literature. Slight differences may come due to the diffferent methods in the *ab initio* approaches of each work, though. The explicitly correlated quantum chemistry approach can be used confidently in order to interpret state-to-the-art experiments relating to molecular clusters.

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REFERENCES

Adler TB, Knizia G, Werner HJ, 2007. A simple and efficient CCSD(T)-F12 approximation. Journal of Chemical Physics, 127. doi: 10.1063/1.2817618.

Albritton DL, Schmeltekop AL, Zare RN, 1979. Potential energy curves for NO+. Journal of Chemical Physics, 71(8). doi: 10.1063/1.438757.

Arthurs AM, Dalgarno A, 1960. The Theory of Scattering by a Rigid Rotator. Proceedings of the Royal Society A, 256: 540–551. doi: 10.1098/rspa.1960.0125.

Boys SF, Bernardi F, 1970. The calculation of small molecular interactions by the differences of separate total energies. Some procedures with reduced errors. Molecular Physics, 19: 553–556. doi: 10.1080/00268977000101561.

Bush AM, Wright TG, Spirko V, Jurek M, 1997. The intermolecular potential energy surface of the Ar·NO^+ cationic complex. Journal of Chemical Physics, 106: 4531. doi: 10.1063/1.473496.

Cernicharo J, Bailleux S, Alekseev E, Fuente A, Roueff E, Gerin M, Tercero B, Treviño-Morales SP, Marcelino N, Bachiller R, 2014. Tentative detection of the nitrosylium ion in space. Astrophysical Journal, 795(1). doi: 10.1088/0004-637X/795/1/40.

Denis-Alpizar O, Stoecklin T, 2015. Rovibrational rate coefficients of NO^+ in collision with He. Monthly Notices of the Royal Astronomical Society, 451: 2986–2990. doi: 10.1093/mnras/stv1137.

Fourré I, Raoult M, 1995. Vibrational structure of the ArNO+ van de Waals cation. Journal of Chemical Physics, 199: 215. doi: 10.1016/0301-0104(95)99001-L.

Halvick P, Stoecklin T, Lique F, Hochlaf M, 2011. Explicitly correlated treatment of the Ar–NO^+ cation. Journal of Chemical Physics, 135(4): 044312. doi: 10.1063/1.3614502.

Herbst E, Klemperer W, 1973. The Formation and Depletion of Molecules in Dense Interstellar Clouds. The Astrophysical Journal, 185. doi: 10.1086/152436.

Hirst DM, 1985. Potential Energy Surfaces: Molecular Structure and Reaction Dynamics. UK: Taylor & Francis group, UK.

Hutson JM, Green S, 2012. MOLSCAT: MOLecular SCATtering v.14. http://adsabs.harvard.edu/abs/2012ascl.soft06004H. (Date of access: 20 June 2018).

Irikura KK, 2007. Experimental vibrational zero-point energies: Diatomic molecules. Journal of Physical and Chemical Reference Data, 36(2). doi: 10.1063/1.2436891.

Knizia G, Adler TB, Werner HJ, 2009. Simplified CCSD(T)-F12 methods: Theory and benchmarks. Journal of Chemical Physics, 130. doi: 10.1063/1.3054300.

Lee EPF, Gamblin SD, Wright TG, 2000. The interaction energies of the Rg·NO cationic complexes: Rg·NO. Chemical Physics Letters, 322: 377. doi: 10.1016/S0009-2614(00)00430-9.

Lee EPF, Soldan P, Wright TG, 1998. Geometries and Binding Energies of Rg·NO^+ Cationic Complexes (Rg=He, Ne, Ar, Kr, and Xe). Journal of Chemical Physics, 102: 6858–6864. doi: 10.1021/jp981696+.

Orek C, Klos J, Lique F, Bulut N, 2016. Ab initio studies of the Rg–$NO^+(X^1\Sigma^+)$ van der Waals complexes (Rg=He, Ne, Ar, Kr, and Xe). Journal of Chemical Physics, 144(20): 204303. doi: 10.1063/1.4950813.

Pickles JB, Williams DA, 1977. Model for surface reactions on interstellar grains - A numerical study. Astrophysics and Space Science, 52(2). doi: 10.1007/BF01093879.

Robbe JM, Bencheikh M, Flament JP, 1993. Ab initio investigation of the ground state potential surfaces of He-NO^+ and Ar-NO^+. Chemical Physics Letters, 210(1–3): 170–174. doi: 10.1016/0009-2614(93)89119-3.

Sato K, Achiba Y, Kimura K, 1984. The Ar-NO van der Waals complex studied by resonant multiphoton ionization spectroscopy involving photoion and photoelectron measurements. Journal of Chemical Physics, 81(57). doi: 10.1063/1.447346.

Si-sheng, W, Rui-hong K, Liu-si S, Li-qing H, Shi-Kang Z, Zhen-ya W, 2007. Theoretical study of RgNO (Rg=He, Ne, Ar and Kr) complexes. Journal of Chemical Physics, 20(113). doi: 10.1360/cjcp2007.20(2).113.6.

Singh PD, Maciel WJ, 1980. On the possibility of the existence of NO^+ in interstellar space. Astrophysics and Space Science, 68(1). doi: 10.1007/BF00641645.

Soldan P, Lee E, Wright T, 2002. The intermolecular potential energy surface of the He·NO^+ cationic complex. Journal of Chemical Physics, 116: 2395. doi: 10.1063/1.1433507.

Stoecklin T, Voronin A, 2011. Vibrational and rotational cooling of NO^+ in collisions with He. Journal of Chemical Physics, 134(204312). doi: 10.1063/1.3590917.

Takahashi M, 1992. Two-color (2+1′) multiphoton ionization threshold photoelectron study of the Ar-NO van der Waals complex: Observation of intermolecular vibrational progressions of the Ar-NO^+ cation. The Journal of Chemical Physics, 96(4). doi: 10.1063/1.462010.

Werner, HJ, Knowles PJ, Knizia G, Manby FR, Schütz M, 2012. Molpro: a general-purpose quantum chemistry program package. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2(2): 242–253. doi: 10.1002/wcms.82.

Wright TG, 1996. Geometric structure of Ar·NO^+: Revisited. A failure of density functional theory. Journal of Chemical Physics, 105: 7579. doi: 10.1063/1.472597.

Wright TG, Spirko V, Hobza P, 1994. Ab initio calculations on Ar-NO+: Structure and vibrational frequencies. Journal of Chemical Physics, 100: 5403–5410. doi: 10.1063/1.467157.