

Collisional quenching of NCO ($A^2\Sigma^+$) by some inorganic molecules

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Abstract

Collisional removal of the $(0,0^0,0)$ level of the $A^2\Sigma^+$ state of the NCO radical has been studied at room temperature (298 K). NCO radicals were produced by laser photolysis of CHBr_3 at 266 nm followed by the reaction of CH with N_2O , then electronically excited with Nd:YAG laser pumped dye laser. The quenching rate coefficients k_q and thermally averaged cross-sections σ_q were determined by the pressure dependence of the time-resolved fluorescence. Colliders investigated are Ar, N_2 , O_2 , CO, NO, N_2O , CO_2 , SO_2 , H_2O and photochemical precursor CHBr_3 . The quenching rates increase on the whole with the increasing of polarities of the colliders. By comparison with the formation cross-sections of complexes calculated by means of a collision complex model, it is believed that the attractive forces play main roles in the collision quenching processes of NCO ($A^2\Sigma^+$) by the quenchers studied in this work.

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1. Introduction

The NCO radical has been suggested as an important intermediate in combustion processes leading to the formation of NO, in particular in the conversion of fuel nitrogen into nitrogen oxides and in the so-called “prompt” NO formation [1,2]. In addition, it plays a role in NO_x reduction processes such as the RAPRENO_x process [3]. So

the kinetic and dynamic studies of the reactions of NCO are of great interest. Since 1980s, the NCO radical has become accessible to spectroscopic detection by laser-induced fluorescence. This has accelerated the studies of NCO reactions. Hancock et al. [4,5] produced NCO radicals directly using IRMPD of PhNCO , or indirectly using IRMPD of CH_2F_2 followed by the reaction of CHF with NO and reported the product dynamics of the $\text{NCO} + \text{NO}$ reaction from time-resolved FTIR emission of the stable products. Perry [6] measured the absolute rate constants for the reactions of NCO radicals with H_2 and NO by 248 nm laser photolysis of HNCO to produce NCO.

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Bimolecular rate coefficients for the reactions of NCO ($X^2\Pi_i$) with some selected unsaturated hydrocarbons were obtained via photolysis of ClNCO–Ar mixtures at 248 nm by Becker et al. [7]. Product branching ratios of the $\text{NCO} + \text{NO}_x$ reactions were studied by Hershberger and Park [8] at room temperature using pulsed photolysis of BrNCO or ICN/ O_2 . The NCO removal rate constants by some unsaturated hydrocarbons and inorganic molecules were measured by Wategaonkar and Setser [9] using the $\text{F} + \text{HNCO}$ reaction system to produce NCO. Atakan and Wolfrum [10] studied the temperature dependence of the reactions of NCO radicals with NO and O_2 by means of the 193 nm laser photolysis of C_2N_2 followed by the reaction of CN with O_2 . Although a quite extensive data set of the reactions of the ground NCO radicals has hitherto been accumulated, only a few are available about the kinetics of excited NCO. Baronavski et al. [11] investigated fluorescence quenching of NCO in CH_4/O_2 and CH_4/air premixed low pressure flames. Fernandez et al. [12] directly measured the removal rates of electronically excited NCO $\text{A}^2\Sigma^+(0,0^0,0)$ by simple molecules by IRMPD of PhNCO to produce NCO coupled with LIF technique.

In this work, NCO was produced via the reaction of CH radicals, generated by 266 nm laser photolysis of CHBr_3 , with N_2O . The quenching rate coefficients of NCO ($\text{A}^2\Sigma^+$) by a group of “standard” collision partners with a variety of properties, as well as precursor CHBr_3 , were obtained by measuring the time-resolved fluorescence signal of the excited NCO at room temperature. That group consists of a kind of inert gases (Ar), two nonpolar diatomics (N_2 and O_2), one nonpolar triatomic (CO_2), three weakly polar molecules (CO, NO, N_2O), and two highly polar molecules (SO_2 and H_2O).

2. Experimental

The experiments were performed using a typical laser photolysis-laser-induced fluorescence (LP-LIF) technique under pseudo-first-order conditions in a flowing reaction vessel made of stainless. Preparation of gases and control of flow velocities

are similar to those employed by Chen and Gao [13,14] and some modifications have been made in this work. Briefly, the parent molecules $\text{CHBr}_3/\text{N}_2\text{O}$ and the quenchers were diluted in a large excess of Ar and stored respectively in 10 l reservoirs prior to experiments. Three gas flows were measured by calibrated mass flow controllers (D07-7A/2M, Beijing): f_1 , the flow of $\text{CHBr}_3/\text{N}_2\text{O}$ in Ar; f_2 , the flow of a quencher mixed with Ar; and f_3 , the flow of pure Ar, which is used to keep the total pressure constant when colliders are added. In all experiments, the gases were slowly flowing through the cell and renewed every 0.1 s, in order to eliminate the kinetic complications caused by the undesired accumulation of photolysis and reaction products. The total pressure P_{total} was about 20 Torr and the partial pressures of CHBr_3 and N_2O in the reaction vessel were about 14 and 60 mTorr, respectively. In our experiments, P_{total} and the partial pressures of CHBr_3 and N_2O were all kept constant.

NCO radical was generated by the reaction of CH with N_2O , where CH radical was produced by the photolysis of CHBr_3 upon the softly focused 266 nm irradiation of a frequency-quadrupled Nd:YAG laser (New wave) operating at 10 Hz. The ground electronic state NCO radical was electronically excited to $\text{A}^2\Sigma^+$ state by a dye laser beam (Lumonics, HD500) pumped by a Nd:YAG laser (Spectra physics, GCR-170, repetition rate of 10 Hz). The photolysis beam and the excitation laser beam propagated in opposite directions through the reactor. In order to reduce laser scattering light, both of them were passed through a set of special light baffles. The fluorescence signal of the excited NCO was detected at right angles to the laser propagation through a cut-off filter with transmitting wavelengths longer than 450 nm before reaching a photomultiplier (GDB56, Beijing). The signal from the photomultiplier was recorded by a transient digitizer, and then averaged with a computer data acquisition system. In our experiment the signal were averaged over 256 laser shots.

Materials. In this work, Ar (99.999%, Nanjing), N_2 (99.999%, Nanjing), O_2 (99.99%, Beijing), CO (99.9%, Nanjing), NO (>99.0%, Beijing), N_2O (99.7%, Beijing), SO_2 (>99.0%, Nanjing) and CO_2 (99.999%, Nanjing) were taken from cylinders

without further purification. CHBr_3 (99.7%, Shanghai) was AR grade and H_2O was distilled and deionized. They were both repeatedly degassed and made up in dilute mixtures with Ar and stored in reservoirs before use.

3. Results and discussion

3.1. Generation of NCO radical

The production of the NCO radicals was established by observing laser-induced fluorescence excitation spectrum of the reaction products in the 434.0–441.5 nm with 15 μs delay time after the 266 nm photolysis of $3.6 \times 10^{14} \text{ cm}^{-3}$ CHBr_3 in the presence of $4.7 \times 10^{15} \text{ cm}^{-3}$ N_2O at 18.7 Torr total pressure. The spectrum is illustrated in Fig. 1, which can be unambiguously assigned to the $\text{X}^2\Pi_i \rightarrow \text{A}^2\Sigma^+$ LIF excitation spectrum of NCO as previously described by Dixon [15].

The mechanism of the 266 nm photolysis of CHBr_3 to produce CH radicals has been studied carefully previously [13]. It is believed that the 266 nm photolysis of CHBr_3 to produce CH radicals includes three steps, each of them is a single-photon absorption process. And in this work, we also obtained CH LIF excitation spectrum in the range of

427–437 nm after 266 nm photolysis of CHBr_3 without the presence of N_2O . The absorption cross-section of N_2O is smaller than $10^{-24} \text{ cm}^2 \text{ molecule}^{-1}$ at 250 nm [16], so it is obvious that the possibility of its photolysis under 266 nm laser irradiation can be ruled out. Therefore it is believed that NCO is one of the products of CH and N_2O reaction system. So far, only one experimental study on the reaction mechanism of the $\text{CH} + \text{N}_2\text{O}$ reaction has been reported by Hersherberger and Hovda [17]. They only observed the $\text{HCN} + \text{NO}$ and $\text{CO} + \text{H} + \text{N}$ channels, and measured the ratio of the two channels as 0.72:0.28 by a time-resolved infrared diode laser absorption technique. We could not establish whether the generation of NCO is direct or indirect presently. A more elaborate experiment is needed to fully elucidate the mechanism of the reaction. However, the measuring of collision rate coefficients for NCO was independent of its mode of generation.

3.2. Time-resolved kinetics

In order to keep the concentration of NCO radical constant, the concentrations of $\text{CHBr}_3/\text{N}_2\text{O}$, the total pressure (circa 20 Torr), and the delay time between the photolysis beam and the exciting laser beam were all kept constant in the whole experiment. Time-resolved NCO fluorescence was observed following excitation at 438.6 nm at the Q subband of the $\text{NCO } \text{A}^2\Sigma^+(0, 0^0, 0) \leftarrow \text{X}^2\Pi_i(0, 0^1, 0)$ transition. The typical decay trace of $\text{NCO } \text{A}^2\Sigma^+$ quenched by H_2O is illustrated in Fig. 2(a). The nature of single exponential decay is demonstrated by the semi-logarithmic plots in Fig. 2(b), where the solid line is the fitting result corresponding to about 100 ns delay from the maximum point in order to reduce the disturbance caused by laser scattering light. Traces were fitted with Eq. (1):

$$I = I_0 \exp(-k't) \quad (1)$$

where k' is the pseudo-first-order rate coefficient accounting for the quenching of NCO ($\text{A}^2\Sigma^+$) by quenchers (k_q) and background gases (k_i), and the Einstein spontaneous emission coefficient of NCO (k_f). In this type of reaction system, background gases include Ar, CHBr_3 , N_2O and some fragments

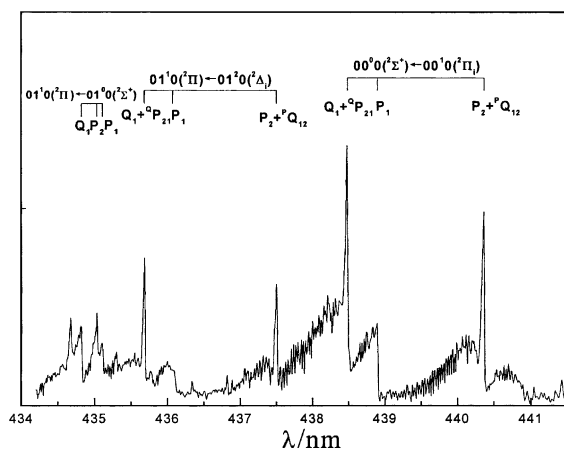


Fig. 1. The low resolution LIF excitation spectrum of NCO. The spectrum was obtained 15 μs after 266 nm photolysis of $3.6 \times 10^{14} \text{ cm}^{-3}$ CHBr_3 in the presence of $4.7 \times 10^{15} \text{ cm}^{-3}$ N_2O in 18.7 Torr argon at 298 K.

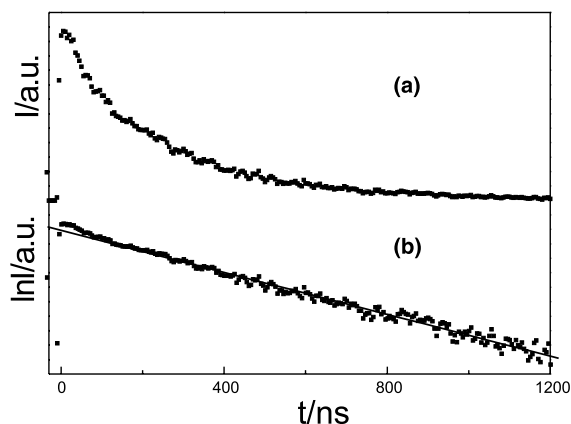


Fig. 2. The typical time-resolved fluorescence decay signal of NCO $A^2\Sigma^+$ quenched by H_2O (a) and its semi-logarithmic plot (b) at 438.6 nm. (■) Experimental data and (—) fitting result.

of photolysis. Therefore, the first-order rate coefficient k' should be expressed as

$$k' = k_q[Q] + \sum_i k_i[M_i] + k_f. \quad (2)$$

In present case, the background gases and total pressure were constant, so the first-order rate coefficient k' increased proportionally to the concentration of the added quenchers, as illustrated in Fig. 3. The second-order quenching rate constants k_q were obtained by linear least-square fitting ac-

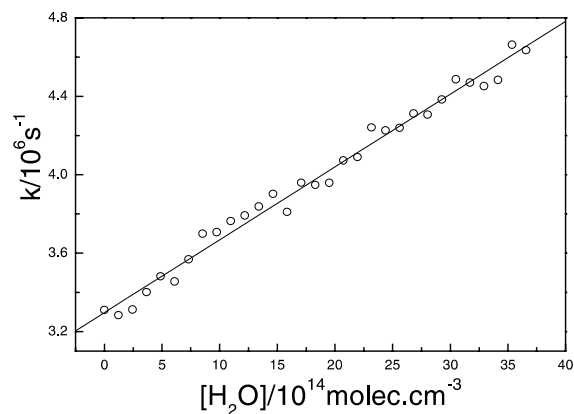


Fig. 3. Plot of the first-order rate constant for quenching of NCO ($A^2\Sigma^+$) as a function of concentration of H_2O .

cording to Eq. (2) from those plots as Fig. 3. The rate constants k_q for the collisional quenching of NCO ($A^2\Sigma^+$) by the selected inorganic molecules at 298 K are summarized in Table 1. As well established, the quenching cross-section σ_q is the function of k_q

$$\sigma_q = k_q/V, \quad (3)$$

where $V = (8kT/\pi\mu)^{1/2}$ is the averaged relative kinetic velocity. Actually, the quenching cross-section σ_q is a synthetic effect, which is related to both collision complex formation process mainly

Table 1

Rate constants k_q and collision cross-sections σ_q for the collisional quenching of NCO ($A^2\Sigma^+$) by the selected inorganic molecules at 298 K

Quencher	P_{total} (Torr)	k_q (10^{-10} cm ³ molecule ⁻¹ s ⁻¹)	σ_q (10^{-2} nm ²)	Ref.
CHBr ₃	20	4.98 ± 0.29	119 ± 7	This work
Ar	≤ 40	$(5.65 \pm 0.31) \times 10^{-3}$	0.10 ± 0.01	This work
	≤ 7	$< 2.0 \times 10^{-3}$		[12]
N ₂	20	0.54 ± 0.03	8.81 ± 0.52	This work
	1	0.21 ± 0.02		[12]
O ₂	20	0.98 ± 0.04	16.6 ± 0.7	This work
	1	0.85 ± 0.04		[12]
CO ₂	20	1.08 ± 0.03	19.9 ± 0.6	This work
	1	0.65 ± 0.02		[12]
CO	20	1.76 ± 0.03	28.7 ± 0.5	This work
N ₂ O	20	2.51 ± 0.16	46.3 ± 3.0	This work
	1	1.52 ± 0.02		[12]
NO	20	3.68 ± 0.14	61.3 ± 2.3	This work
	1	3.20 ± 0.3		[12]
H ₂ O	20	3.71 ± 0.08	52.4 ± 1.1	This work
SO ₂	20	5.20 ± 0.17	104 ± 3	This work
	1	2.71 ± 0.1		[12]

due to the long-range interaction between the collision partners and the formation probability of the quenching products from the complex. Hence, the collision cross-sections σ_q were also obtained and summarized in Table 1. The uncertainty of k_q corresponds to one standard deviation from linear least-square fitting, and the uncertainty of σ_q is derived from the uncertainty of k_q .

3.3. Discussion

The kinetic studies of NCO ($A^2\Sigma^+$) in collisions with some small molecules have been investigated previously only by Fernandez et al. [12] and they have analyzed and discussed the results in terms of the correlation with the potential well depth of the collision partners. Although the generation of NCO radicals is different, the results presented here are in satisfactory agreement with previous study as shown in Table 1. The rate constants presented here for NCO ($A^2\Sigma^+$) clearly refer to the total removal rate for this excited species by both physical quenching and reaction channels. Strictly therefore, our data provide only upper limits to the rate constants for chemical reaction. Apart from a very few publication about the collisional quenching processes of electronically excited NCO radicals by the selected inorganic molecules presented here could be found, there have been many studies made for NCO ($X^2\Pi_i$). The ground state and the first excited state of NCO have the same molecular point group, it is interesting therefore to compare the present data with those data about NCO ($X^2\Pi_i$).

No publication about the collisional quenching processes of electronically excited NCO radicals by CHBr_3 precursor could be found. In this work, the total pressure was kept constant and only the partial pressure of CHBr_3 was varied. The results in Table 1 demonstrate clearly that the collisional quenching of NCO ($A^2\Sigma^+$) by CHBr_3 is very effective.

It is the fact that argon is an inefficient quencher for NCO ($A^2\Sigma^+$). And in this work, the variation in Ar pressure was within 40 Torr, which is much larger than that in [12], resulting in a variation in the pseudo-first-order rate constant of NCO ($A^2\Sigma^+$) decay to be a small value compared with

the decay rate itself. Therefore, a significant error may be caused. The magnitude of the quenching rate constant of NCO ($A^2\Sigma^+$) by Ar, however, seems reasonable.

The quenching of NCO ($A^2\Sigma^+$) by N_2 or O_2 is also inefficient. The two quenching rate constants have the upper limit of $10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. The values that we obtained are in fairly agreement with the results reported by Fernandez et al. [12], with an exception of somewhat larger. Actually, the reactions of the ground state of NCO with N_2 or O_2 have been more extensively studied. As for NCO ($X^2\Pi_i$), N_2 cannot react with it at 298 K, so as to be used as buffer gas [10]. As for the reaction of NCO ($X^2\Pi_i$) + O_2 , those authors estimated the bimolecular rate constant at room temperature is in the range of 10^{-16} – $10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ [10,18]. However, the trend of increasing of $k_{\text{NCO} (X^2\Pi_i) + \text{O}_2}$ with temperature in the range 296–749 K was investigated by Becher et al. [19].

The quenching rate constants of NCO ($A^2\Sigma^+$) by CO and CO_2 obtained in this work are also comparatively small. The earlier study of NCO ($A^2\Sigma^+$) quenched by CO_2 , using IRMPD of PhNCO to generate NCO (X), also gave good agreement. Although the mass and volume of the CO molecule is smaller than that of CO_2 , the collisional quenching rate constant of NCO ($A^2\Sigma^+$) by CO is faster than that by CO_2 . The reason for this is probably that CO is a polar molecule, however, CO_2 , which has linear symmetry, is a nonpolar molecule and its dipole moment is zero. As for the reactions of the ground state of NCO, the value of $(1.0 \pm 0.8) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with CO at 298 K and 100 Torr total pressure, and the upper limit of $<1.0 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with CO_2 at 298 K and 20 Torr total pressure, were also obtained [19].

The collisional quenching of NCO ($A^2\Sigma^+$) by NO and N_2O have also been reported [12]. And it is obvious that NO and N_2O are more efficient in quenching of NCO ($A^2\Sigma^+$). They are both weakly polar molecules, and the mass and volume of the N_2O molecule are bigger than those of NO. However, it is interesting to find that the collisional quenching rate constant of NCO ($A^2\Sigma^+$) by NO is faster than that by N_2O , and Fernandez et al. [12] observed the same phenomenon. It is

probably that they have different reaction mechanisms. Actually, no evidence could be seen of reactive removal of the ground state NCO by N₂O [4,17]. However, the NO + NCO (X²Π_i) reaction have been reported by many groups, and the value of $3.4 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the reaction has been accepted [4,6,10]. It is believed that the NO + NCO (X²Π_i) reaction should have no activation energy and should react on an attractive potential energy surface to the ON–NCO complex at low temperatures.

CO₂, N₂O, H₂O, and SO₂ are all triatomic molecules, but the collisional quenching rate constants are considerably different from each other, which increase in the sequence of CO₂, N₂O, H₂O, and SO₂. It is well known that N₂O, H₂O, and SO₂ have the same symmetry (C_{2v}) with the exception of CO₂, which has C_{∞v} symmetry. The polarity of the four kinds of molecules increases in the sequence of CO₂, N₂O, SO₂, and H₂O. Although the polarity of H₂O is higher than that of SO₂, the mass and volume of H₂O is smaller than that of SO₂. It is indicated that the attractive forces between the excited NCO radical and CO₂, N₂O, H₂O, and SO₂ molecules are

probably important in the collision quenching processes of the excited NCO radical by these molecules.

In order to obtain some insight into the collision mechanism between NCO (A²Σ⁺) and the selected collision partners, we also calculated the formation cross-sections of the radical adducts of NCO (A²Σ⁺) with the selected inorganic molecules by using the collision complex model proposed by Fairchild et al. [20]. According to the theory, the long-range part of the interaction between the excited state of molecules and the collision partners is composed of a sum of attractive multipole interactions (dipole–dipole, dipole–quadrupole, dipole–induced dipole, and dispersion) and a repulsive centrifugal barrier. Thus, the effective potential could be expressed using the most favorable orientation method as

$$V_{\text{eff}} = Eb^2/r^2 - C_3/r^3 - C_4/r^4 - C_6/r^6 \quad (4)$$

or the averaged orientation method [21]

$$V_{\text{eff}} = Eb^2/r^2 - C'_6/r^6 - C_8/r^8. \quad (5)$$

Table 2

Summary of the measured quenching rate constants σ_q , the calculated formation cross-sections σ_{eff} and the parameters used in the calculations at 298 K

Quencher	μ^a (D)	α^a (Å ³)	Q^b (10 ^{−26} esu cm ²)	IP ^a (eV)	σ_q (10 ^{−2} nm ²)	Maximum ^d		Average ^c	
						σ_{eff}	P	σ_{eff}	P
CHBr ₃	0.99	11.8	3.40	10.48	119 ± 7	149	0.80	121	0.98
Ar	0.00	1.64	0.00	15.76	0.10 ± 0.01	65.4	0.002	65.3	0.002
N ₂	0.00	1.74	1.52	15.58	8.81 ± 0.52	71.1	0.12	66.7	0.13
O ₂	0.00	1.58	0.39	12.07	16.6 ± 0.7	63.5	0.26	62.1	0.27
CO	0.11	1.95	2.50	14.01	28.7 ± 0.5	79.3	0.36	68.7	0.40
CO ₂	0.00	2.91	4.30	13.77	19.9 ± 0.6	88.3	0.23	78.7	0.25
NO	0.16	1.70	1.80	9.26	61.3 ± 2.3	73.2	0.84	61.6	0.99
N ₂ O	0.16	3.03	3.00	12.89	46.3 ± 3.0	90.8	0.51	78.6	0.59
SO ₂	1.63	3.72	4.40	8.87	104 ± 3	139	0.75	89.6	1.16
H ₂ O	1.85	1.45	0.13	12.62	52.4 ± 1.1	129	0.41	80.5	0.65
NCO (A)	0.45 ^c	3.00 ^f	3.50 ^f	10.17 ^g					

^a Ref. [22].

^b Refs. [23,24].

^c Calculated using the averaged orientation method.

^d Calculated using the most favorable orientation method.

^e Calculated using CIS/6-311++G(d,p) method.

^f Estimated following [25].

^g Calculated using MP2/6-311++G(d,p) method.

The C_n coefficients may be expressed in terms of the dipole and quadrupole moments, polarizability and ionization potential of excited NCO and the collision partner. In a collision at a particular kinetic energy E , there exists an impact parameter b_0 where the maximum of the effective potential is just equal to E and only for $b < b_0$, the collision pair can form a complex. Following this method, we can obtain the thermally averaged complex formation cross-section at temperature T . The results of the calculations at the temperature of 298 K, the parameters used in the calculations and the experimentally measured quenching cross-sections are summarized in Table 2.

According to [20], the cross-section for quenching is that for complex formation times a probability P that quenching will occur during the residence time of the complex, viz. $\sigma_q = P\sigma_{\text{eff}}$. Actually, we have no way of knowing P a priori, or how it varies among collision partners. From the results listed in Table 2, it is obvious that the probability P should be different for different quenchers. When the collision partners are Ar molecules, the probability of forming quenching products almost equals to zero. As for the other collision partners, it should be different for different quenchers and generally less than 1. However, in respect that this simple one-dimensional collision calculation is a very approximate version of the actual dynamics of such complex formation and the parameters NCO ($A^2\Sigma^+$) used in the calculations were not very precise for the lack of the precise values, it is suggested that the comparison about σ_{eff} and P be more applicable qualitatively than quantitatively. When the value of P is around 1.0, it only means that the quencher is very effective.

4. Conclusion

A group of rate constants for quenching of NCO radical in electronically excited states by the selected inorganic molecules has been obtained in the current study and are consistent with the results published previously. It is shown that the quenching rate increase with the polarity of the

collision partners roughly. By using a collision complex model based on attractive forces we estimated complex formation cross-sections. It is indicated that attractive forces and collision complex formation play an important role in the quenching of electronically excited NCO radicals by the selected inorganic molecules as the calculated results are in qualitative agreement with the experimental results.

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