International Journal of Mass Spectrometry 223–224 (2003) 403–409

www.elsevier.com/locate/ijms

A temperature-dependent selected ion flow tube study of anions reacting with SF_5CF_3

Susan T. Arnold[a,*], Thomas M. Miller[a], A.A. Viggiano[a], Chris A. Mayhew[b]

[a] *Air Force Research Laboratory, Space Vehicles Directorate, 29 Randolph Rd, Hanscom AFB, MA 01731-3010, USA*
[b] *Molecular Physics Group, School of Physics and Astronomy, University of Birmingham, Edgbaston, Birmingham B15 2TT, UK*

Received 9 January 2002; accepted 24 May 2002

Abstract

Rate constants and product distributions were measured for the reactions of trifluoromethyl sulfurpentafluoride (SF_5CF_3) with 11 anions using two selected ion flow tube instruments. The reaction of O_2^- was studied from 240 to 500 K and was found to proceed at approximately 30% of the collisional rate, yielding SF_5^- as the only product ion, presumably via a dissociative electron transfer mechanism. The reaction of OH^- proceeds predominantly via nucleophilic attack at the carbon atom, displacing SF_5^- at approximately 25% of the collisional rate at 298 K. The rate constant exhibits a $T^{-1.8}$ dependence from 240 to 500 K, suggesting the reaction occurs through a long-lived collision complex. The F^- reaction, which proceeds at 70% the collisional rate at 298 K, also occurs via nucleophilic attack at the carbon atom, leading to the SF_5^- product ion. The O^- ion reacts predominately by nucleophilic attack at the carbon atom and also via CF_3 radical transfer to O^-. The product branching fraction for the O^- reaction did not vary with temperature, although the rate constant exhibits a $T^{-1.6}$ dependence, similar to that of the OH^- reaction. The ions SF_6^-, CF_3^-, NO_2^-, CO_3^-, Cl^-, NO_3^-, and SF_5^- were found to be unreactive toward SF_5CF_3, despite the fact that sufficiently exothermic reactive channels exist for many of these ions. (Int J Mass Spectrom 223–224 (2003) 403–409)
Published by Elsevier Science B.V.

Keywords: Trifluoromethyl sulfurpentafluoride; SIFT; Anion kinetics

1. Introduction

A GC-MS analysis of stratospheric air samples by Sturges et al. [1] has indicated that trifluoromethyl sulfurpentafluoride (SF_5CF_3) is present in the stratosphere. The compound is thought to be exclusively anthropogenic in origin; Sturges et al. speculate that the source of atmospheric SF_5CF_3 may be the reaction of SF_6 with fluoropolymers in electrical devices. Although present at a level of only 0.12 ppt in 1999, the atmospheric abundance of SF_5CF_3 is reportedly increasing by 6% per year, tracking the increase of atmospheric SF_6. This is significant because both SF_6 and SF_5CF_3 are powerful greenhouse gases. The global warming potential (GWP) of SF_5CF_3 is currently estimated at 18,000 times that of CO_2, making it one of the largest of any molecules.

The stratospheric profile that was measured by Sturges et al. suggests this compound is long-lived in the atmosphere. We have recently speculated that, because the compound is not broken down by UV photodissociation [2] and there are no known atmospheric

---

[*] Corresponding author. E-mail: susan.arnold@hanscom.af.mil

1387-3806/02/$ – see front matter. Published by Elsevier Science B.V.
PII S1387-3806(02)00929-6

sinks, ion–molecule reactions and electron attachment reactions will play a significant role in the atmospheric chemistry of SF_5CF_3. Previous reports from our laboratories on the electron attachment rate to SF_5CF_3 place an upper limit of 1000 years on the compound's atmospheric lifetime [3,4].

As a further exploration of this molecule, Miller et al. [4] have performed ab initio calculations on SF_5CF_3 and its corresponding anion, obtaining equilibrium structures, an electron affinity (EA), and neutral and anion bond dissociation energies and heats of formation. Kennedy and coworkers [5,6] have reported on the reactions of SF_5CF_3 with a variety of cations of atmospheric and industrial importance. In this paper, we continue our investigations of SF_5CF_3, reporting the first negative ion chemistry of this molecule. We present temperature-dependent rate coefficients and product ion distributions for the reactions of SF_5CF_3 with several anions of atmospheric importance. Because of the anthropogenic nature of this compound and the speculation that it may be formed in industrial processes, we have also examined the reactions of SF_5CF_3 with several anions of industrial importance.

2. Experimental

Measurements were made using two separate selected ion flow tube (SIFT) instruments, one at the Air Force Research Laboratory (AFRL) and one at the University of Birmingham (UB). Both of these instruments, as well as the technique, have been described previously in detail [7–9]. Therefore, only a brief description of the method and details pertinent to the present study are given here. In each apparatus, the reactant ions were formed in a remote ion source region and were mass selected using a quadrupole mass spectrometer. The ions were then injected into the flow tube through a Venturi inlet into a fast flow of Helium buffer gas ($\sim 100\,\mathrm{m\,s^{-1}}$ of He, 99.997%). The flow tube pressure was maintained at 0.45–0.5 Torr; the flow tube temperature was maintained at 298 K in the UB instrument, and it was varied from 240 to 500 K in the AFRL instrument. The SF_5CF_3 reactant was introduced downstream through an inlet entering the flow tube perpendicular to the flow. The lower temperature limit in the AFRL measurements was chosen to avoid freezing SF_5CF_3 in the inlet line. A small fraction of the gas in the tube flowed through a sampling orifice, and the reactant and product ions in this flow were mass analyzed using a second quadrupole mass spectrometer. Rate constants were determined by recording the semi-logarithmic decrease in the reactant ion signal as a function of the SF_5CF_3 flow rate. The accuracy of the rate constants measured at AFRL is ±25% with a relative accuracy of ±15%, and the accuracy of the rate constants measured at UB is ±20%. Product branching fractions were determined by monitoring the fractional product ion signal intensities as a function of the SF_5CF_3 flow rate. Extrapolation to a neutral reactant flow rate of zero yields the branching fractions for the primary reaction. Uncertainties in the product distributions are considered to be 5% points.

In the UB apparatus, reactant ions were generated in a high pressure (ca. several Torr) electron impact ion source containing an appropriate precursor gas: O_2 for O_2^-; N_2O/CH_4 for OH^-; SF_6 for SF_5^-; C_2F_6 for F^- and CF_3^-; and CH_3Cl for Cl^-. In the AFRL apparatus, reactant ions were produced using a supersonic expansion ion source [10] with the following precursor gases: O_2 for O^- and O_2^-, O_2/H_2O for OH^-; CO_2/air for CO_3^-; HNO_3/O_2 for NO_2^- and NO_3^-. Samples of the SF_5CF_3 reactant gas were obtained commercially by UB from Apollo Scientific Limited (Derbyshire, UK) and by AFRL from Oakwood Products (South Carolina, USA) and were used without further purification. The stated purity of the commercial samples was 99%.

3. Results

Reaction rate constants and product branching fractions are shown in Table 1 for 11 anions of atmospheric or industrial plasma importance reacting with SF_5CF_3. The reactions are ordered according to the corresponding neutral atom or molecule's EA. Note for comparison that the EA of SF_5CF_3 has been

Table 1
Measured reaction rate constants, k_2, calculated collisional rate constants, k_c (both in units of 10^{-9} $cm^3\,s^{-1}$), product distributions, and reaction exothermicities, Δ_rH (in $kJ\,mol^{-1}$) for various anions reacting with SF_5CF_3

EA	Ion	Products	Δ_rH	Temperature (K)	k_2 UB	k_2 AFRL	k_c
0.44	O_2^-	$SF_5^- + (CF_3 + O_2)$	−35	240		0.47	1.51
				298	0.36	0.55	1.49
				400		0.41	1.48
				500		0.43	1.47
1.05	SF_6^-	n.r.		298	<0.0001		0.86
1.46	O^-	$SF_5^- + CF_3O$ (87%)	−381	240		0.90	2.05
		$CF_3O^- + SF_5$ (3%)	−382	298		0.67	2.04
		$F^- + (SF_5 + CF_2O)$ or	−209	400		0.39	2.02
		$(SOF_4 + CF_3)$ (10%)	−69	500		0.29	2.00
1.83	OH^-	$SF_5^- + CF_3OH$ (100%)	−411	240		0.63	2.00
				298		0.53	1.98
				400		0.25	1.96
				500		0.18	1.95
1.83	OH^-	$SF_5^- + CF_3OH$ (94%)	−411	298	0.44		1.98
		$CF_3^- + SF_5OH$ (6%)[a]	−85				
1.84	CF_3^-	n.r.		298	<0.0001		1.10
2.30	NO_2^-	n.r.		298		<0.006	1.28
3.3	CO_3^-	n.r.		298		<0.006	1.16
3.40	F^-	$SF_5^- + CF_4$	−302	298	1.3		1.88
3.62	Cl^-	n.r.		298	<0.0001		1.44
3.92	NO_3^-	n.r.		298		<0.006	1.14
4.2	SF_5^-	n.r.		298	<0.0001		0.89

The notation “n.r.” indicates no reaction products were detected, and an upper limit to the rate constant is given. Neutral products are assumed based on mass conservation and thermodynamic considerations. UB and AFRL indicate measurements made at the University of Birmingham and the Air Force Research Laboratory, respectively. The electron affinity (EA) of the reactant ion’s corresponding neutral (in eV) taken from [11,19].

[a] 298 K measurements of OH^- reaction at UB identified a 6% CF_3^- product channel, which was not observed in any of the AFRL temperature-dependent measurements.

calculated to be 1.24 eV [4]. The rate constants listed in Table 1 represent an average of two to six independent measurements. The notation “n.r.” indicates no reaction products were detected; an upper limit to the rate constant is reported for those reactions, based on the limitations of the SIFT instruments. Neutral products of reaction were not detected but were inferred from mass conservation and thermochemical considerations. Enthalpies of reaction were calculated using heats of formation reported from the following sources: SF_5CF_3 ($-1639\,kJ\,mol^{-1}$) from Miller et al. [4]; O^-, O_2^-, OH^-, F^-, CF_4, CF_3, CF_2O, and CF_3O^- from Lias et al. [11]; SF_4 and SF_5 from Irikura [12], SF_5^- from the revised EA of SF_5 reported by Miller et al. [13] and the value of $\Delta_fH(SF_5)$ reported by Irikura [12]; CF_3O from Schneider and Wallington [14]; CF_3O_2 from Vedeneev et al. [15]; and $\Delta_fH(SF_5OH)$ estimated by Herron [16]. A G2 calculation was carried out for CF_3OH, and a value of $-931\,kJ\,mol^{-1}$ was obtained for $\Delta_fH^{\circ}_{298}(CF_3OH)$ using the atomization method and the standard thermal correction procedure. Collisional rate constants were determined by the method of Su and Chesnavich [17] using the experimentally determined dipole moment of 0.384 D reported by Malmberg and Maryott [18] and an estimated polarizability of 10.0 $Å^3$, which is exactly intermediate to those of $(SF_5)_2$ and $(CF_3)_2$ [19].

Two of the reactions reported here were studied at both UB and AFRL, namely the reactions of O_2^- and OH^- at 298 K. In both cases, the rate constants measured at AFRL were larger; however, within the combined uncertainties of the two measurements, the values are in agreement. Both laboratories found that SF_5^- is the only product ion of the O_2^- reaction. For

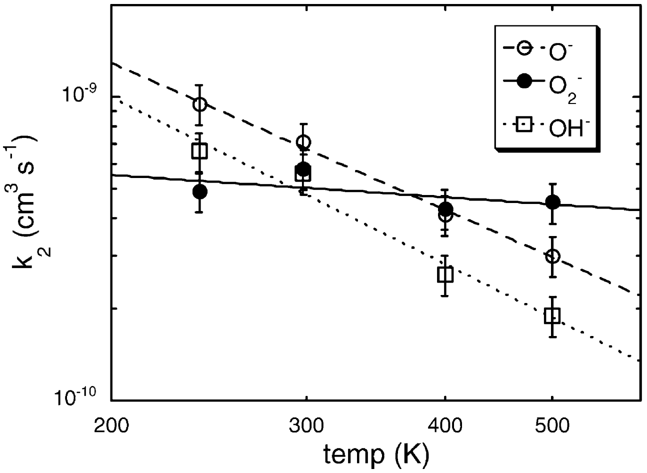

Fig. 1. Temperature-dependent rate constants for the reactions of O_2^-, O^-, and OH^- with SF_5CF_3. The O_2^- reaction has, at best, a weak temperature-dependence ($T^{-0.2}$), while the temperature dependences of the O^- and OH^- reactions are $T^{-1.6}$ and $T^{-1.8}$, respectively.

the OH^- reaction, measurements at AFRL indicate SF_5^- is the sole product ion from 240 to 500 K while the 298 K measurements at UB indicate there is an additional minor product channel (6%) corresponding to the formation of CF_3^-. This difference remains unresolved even after measurements were repeated at a later date.

Measurements for most reactions were made only at 298 K; however, three reactions were studied as a function of temperature from 240 to 500 K. The temperature-dependent rate constants for the reactions of O_2^-, O^-, and OH^- with SF_5CF_3 are plotted in Fig. 1. The O_2^- reaction has, at best, a weak temperature dependence ($T^{-0.2}$), although within the relative uncertainties of the measurements, there may be no temperature dependence at all. The product distributions for the O_2^-, O^-, and OH^- reactions exhibited no temperature dependence from 240 to 500 K.

4. Discussion

4.1. O_2^-

The reaction of O_2^- with SF_5CF_3 proceeds at approximately 30% of the collision rate, yielding SF_5^- as the only product ion. Excluding the 298 K measurement, the temperature dependence of the rate constant from 240 to 500 K mirrors that of the collision rate, meaning the reaction remains ∼30% efficient throughout this temperature range. The likely reaction mechanism is dissociative electron transfer, although we cannot rule out the possibility of a chemically reactive channel, producing CF_3O_2 neutral, since that channel is sufficiently exothermic (190 kJ mol^{-1}). We favor the dissociative electron transfer mechanism because (1) chemically reactive channels that are exothermic and also proceed at a fraction of the collision rate typically display a steeper negative temperature dependence [20] and (2) there are remarkable similarities between this reaction and the electron attachment process that we reported on earlier.

We have previously reported that attachment of thermal electrons to SF_5CF_3 also proceeds at approximately 30% of the maximum rate and yields only SF_5^- products [3,4]. The parent anion, $SF_5CF_3^-$, was not observed in the attachment studies, and this was found to be consistent with calculations that indicated the lowest energy structure of the parent anion is an ion–molecule complex of the form $SF_5^-(CF_3)$ which has a relatively weak D°_{298}[S–C] of only 22 kJ mol^{-1}

[4]. Such a weakly bound complex, if formed upon electron attachment or electron transfer, is likely to dissociate in the relatively high pressure environment of a flow tube, although it may survive in a low temperature ICR experiment. The similarity between the processes of electron attachment and electron transfer suggests the initial electron transfer is the rate-limiting step in the reaction of O_2^- with SF_5CF_3.

4.2. O^-, OH^-, F^-

The only other anions in this survey that were found to react with SF_5CF_3 are O^-, OH^-, and F^-. For all three ions, the dissociative and non-dissociative electron transfer reactions with SF_5CF_3 are significantly endothermic, indicating that the observed product ions must result from chemically reactive pathways.

The reaction of OH^- with SF_5CF_3, which proceeds at approximately 25% of the collision rate at 298 K, primarily occurs via nucleophilic attack at the carbon atom:

$$OH^- + SF_5CF_3 \rightarrow SF_5^- + CF_3OH \quad (1)$$

The reaction proceeds at only a fraction of the collisional rate, and the rate constant exhibits a $T^{-1.8}$ dependence over the range from 240 to 500 K. It is not uncommon for rate constants of exothermic ion–molecule reactions to exhibit a negative temperature-dependence when the reactions are inefficient [20]. This is often interpreted as an indication that the reaction occurs through a long-lived collision complex, and a higher collision energy simply facilitates back decomposition of the complex into reactants.

The appearance of a minor CF_3^- product channel in the OH^- reaction, as observed in the UB measurements, suggests nucleophilic attack may also occur at the sulfur atom. The $CF_3^- + SF_5OH$ product channel is approximately 85 kJ mol^{-1} exothermic, and CF_3^- fragment ions have been reported from a recent non-thermal electron attachment study of SF_5CF_3 [21]. The CF_3^- product ion was not observed in any of the AFRL temperature-dependent measurements of the OH^- reaction. Thus, although a CF_3^- product may indeed form from the reaction of OH^- with SF_5CF_3 under higher energy conditions than were examined in this study, we cannot rule out the possibility that the current observation of CF_3^- product ions results from reaction with an unidentified impurity species in the SF_5CF_3 sample used at UB. The stated impurity of the sample obtained from the manufacturer is 1%; however, the reaction of OH^- with SF_5CF_3 proceeds at less than the collisional rate, meaning a fast reacting impurity could account for the minor CF_3^- product. Although the two laboratories used different source methods to prepare the OH^- reactant ion, this is not likely to explain the difference in the reported product distributions because there are no other ions at an m/q of 17 that could reasonably be produced from the available source gases and formation of excited state species is generally not an issue with molecular anions.

The reaction of F^- with SF_5CF_3 appears to occur exclusively via nucleophilic attack at the carbon atom, yielding SF_5^- as the only product ion. The reaction proceeds at 70% of the collisional rate at 298 K, an efficiency that is significantly higher than was observed for the related reactions of F^- with the trifluoromethyl halides, CF_3X ($X = F, Cl, Br, I$). Morris [22] has previously reported that the efficiency of the nucleophilic displacement reaction

$$F^- + CF_3X \rightarrow X^- + CF_4 \quad (2)$$

increased as X became a better leaving group. The ability of a group to function as a leaving group in a nucleophilic displacement reaction is related to its basicity; generally if a group is a weak base, it will be a good leaving group. In terms of leaving group ability, $I > Br > Cl > F$. Because SF_5 would be considered a very weak base compared to the halogen atoms, it may not be surprising that the efficiency of the nucleophilic displacement reaction of F^- with SF_5CF_3 is much greater than was observed for the corresponding trifluoromethyl halides.

The O^- anion also reacts with SF_5CF_3 predominantly by nucleophilic attack at the carbon atom, yielding SF_5^- product ions and neutral CF_3O. The efficiency of the nucleophilic displacement channel is approximately 30%, which is comparable to that of the OH^- reaction with SF_5CF_3. The reaction channel that yields the CF_3O^- product ion and SF_5 neutral results from CF_3 radical transfer to O^-. This channel has the same exothermicity as the nucleophilic displacement channel; however, it is only a minor product channel. The mechanism accounting for the F^- product channel is somewhat more difficult to characterize. Although thermodynamic arguments alone cannot distinguish whether the mechanism involves attack at the carbon atom and/or the sulfur atom, since both are exothermic processes, we prefer the carbon atom attack because (1) the CF_3O^- product ions can be formed initially with sufficient internal energy that subsequent dissociation of the product ion into F^- and CF_2O is feasible [23] and (2) there is presumably more steric hindrance associated with a sulfur atom attack. Interestingly, the product branching fraction for the O^- reaction was not found to vary with temperature, although the rate constant exhibits a $T^{-1.6}$ dependence, similar to that of the OH^- reaction. As mentioned above, this kind of temperature dependence on the rate constant is generally interpreted as an indication that the reaction occurs through a long-lived collision complex. While an increase in temperature is expected to affect the dissociation dynamics of the collision complex, it does not appear to affect the final product distribution of the O^- reaction.

4.3. SF_6^-, CF_3^-, NO_2^-, CO_3^-, Cl^-, NO_3^-, SF_5^-

The ions SF_6^-, CF_3^-, NO_2^-, CO_3^-, Cl^-, NO_3^-, and SF_5^- are all found to be unreactive toward SF_5CF_3. For the SF_6^- reactant, the only exothermic reaction channel is non-dissociative electron transfer; however, the molecular anion, $SF_5CF_3^-$, has never been observed. It is not formed in low energy electron attachment to SF_5CF_3 [3,4,21]. The dissociative electron transfer channel, forming $SF_5^- + CF_3 + SF_6$, is endothermic by only 4 kJ mol^{-1}. However, even very exothermic charge transfer reactions involving SF_6^- have been found to be slow [20], a fact generally attributed to the large geometry difference between SF_6 and SF_6^-. Other potential product channels are also endothermic, which explains the observed lack of reactivity with SF_6^-.

Electron transfer to SF_5CF_3 is endothermic for the CF_3^-, NO_2^-, CO_3^-, Cl^-, NO_3^-, and SF_5^- reactants. Several of these ions do have potential chemically reactive channels that are significantly exothermic; however, none were observed, despite the apparent similarity with some previously discussed reactions. For example, the nucleophilic displacement channel involving the Cl^- reactant

$$Cl^- + SF_5CF_3 \rightarrow SF_5^- + CF_3Cl \qquad (3)$$

is exothermic by 100 kJ mol^{-1}, and the similar reaction with F^- was found to proceed with an efficiency of approximately 70%, yet reaction 3 is not observed. The Cl^- ion is generally less reactive than F^- [20]; however, rather large difference observed here suggests there may be a significant barrier associated with the SF_5CF_3 nucleophilic displacement channel possibly due to more steric hindrance associated with Cl^- attack at the carbon atom than is the case with F^-. This may also explain why the nucleophilic displacement with the CF_3^- reactant does not occur despite the large exothermicity:

$$CF_3^- + SF_5CF_3 \rightarrow SF_5^- + C_2F_6, \quad \Delta_f H = -312\,\mathrm{kJ\,mol^{-1}} \qquad (4)$$

Because F^- transfer was not observed to SF_5CF_3 from either SF_6^-, SF_5^-, or CF_3^- reactant ions, an upper limit of 160 kJ mol^{-1} is placed on the fluoride affinity of SF_5CF_3.

5. Conclusion

Rate constants and product ion distributions are reported for the reactions of O_2^-, O^-, OH^-, and F^- with SF_5CF_3. The F^- reaction proceeds with an efficiency of approximately 70%. The O_2^-, O^-, and OH^- reactions all proceed at 25–30% of the collisional rate at 298 K. The rate constant for the O_2^- reaction exhibits essentially no temperature dependence, while the rate constants for the O^- and OH^- reactions exhibit temperature dependences similar to one another, $T^{-1.6}$ and $T^{-1.8}$, respectively. The likely mechanism of the O_2^- reaction is dissociative electron transfer, which yields SF_5^- as the only product ion. Electron transfer channels are endothermic for the O^-, OH^-, and F^- reactions, indicating the observed reaction products result from chemically reactive pathways. The OH^- and F^- reactions proceed via nucleophilic attack at the carbon atom, yielding SF_5^- product ions. There are at least two mechanisms evident in the O^- reaction, the dominant mechanism being nucleophilic attack at the carbon atom, and the minor channel being CF_3 radical transfer to O^-. The ions SF_6^-, CF_3^-, NO_2^-, CO_3^-, Cl^-, NO_3^-, and SF_5^- were all found to be unreactive toward SF_5CF_3 despite the fact that sufficiently exothermic reactive channels exist for many of these ions.

The present results demonstrate that SF_5CF_3 does not react with the dominant negative ions in the lower atmosphere, namely CO_3^- and NO_3^-. A reaction is observed between SF_5CF_3 and O_2^-, an ion that is present in the atmosphere at slightly higher altitudes. However, the slow rate constant associated with the O_2^- reaction suggests it will play no role in the atmospheric chemistry of SF_5CF_3.

Acknowledgements

CAM is grateful for the assistance of Ms. C. Atterbury during the SIFT measurements and acknowledges financial support provided by the UK Technological Plasma Initiative Program, EPSRC, under Grant Reference GR/L82083. The AFRL authors acknowledge technical support provided by John Williamson and Paul Mundis and financial support provided by the US Air Force Office of Scientific Research under Project no. 2303EP4. T.M.M. was supported through Visidyne Inc. (Burlington, MA) under contract number F19628-99-C-0069.

References

[1] W.T. Sturges, T.J. Wallington, M.D. Hurley, K.P. Shine, K. Sihra, A. Engel, D.E. Oram, S.A. Penkett, R. Mulvaney, C.A.M. Brenninkmeijer, Science 289 (2000) 611.

[2] R.Y.L. Chim, R.A. Kennedy, R.P. Tuckett, W. Zhou, G.K. Jarvis, D.J. Collins, P.A. Hatherly, J. Phys. Chem. A 105 (2001) 8403.

[3] R.A. Kennedy, C.A. Mayhew, Int. J. Mass Spectrom. 206 (2001) i.

[4] T.M. Miller, S.T. Arnold, A.A. Viggiano, W.B. Knighton, J. Chem. Phys. 116 (2002) 6021.

[5] C. Atterbury, R.A. Kennedy, C.A. Mayhew, Phys. Chem. Chem. Phys. 3 (2001) 1949.

[6] C. Atterbury, A.D.J. Critchley, R.A. Kennedy, C.A. Mayhew, R.P. Tuckett, Phys. Chem. Chem. Phys. 4 (2002) 2206.

[7] D. Smith, N.G. Adams, Adv. At. Mol. Phys. 24 (1988) 1.

[8] N.G. Adams, D. Smith, in: J.M. Farrar, W.H. Saunders Jr. (Eds.), Techniques for the Study of Ion–Molecule Reactions, Wiley, New York, 1988, p. 165.

[9] A.A. Viggiano, R.A. Morris, F. Dale, J.F. Paulson, K. Giles, D. Smith, T. Su, J. Chem. Phys. 93 (1990) 1149.

[10] S.T. Arnold, R.A. Morris, A.A. Viggiano, M.A. Johnson, J. Phys. Chem. 100 (1996) 2900.

[11] S.G. Lias, J.E. Bartmess, J.F. Liebman, J.L. Holmes, R.D. Levin, W.G. Mallard, in: W.G. Mallard, P.J. Linstrom (Eds.), NIST Chemistry WebBook, NIST Standard Reference Database Number, Gaithersburg (http://webbook.nist.gov), 1998, p. 69.

[12] K.K. Irikura, J. Chem. Phys. 102 (1995) 5357.

[13] A.E.S. Miller, T.M. Miller, A.A. Viggiano, R.A. Morris, J.M.V. Doren, S.T. Arnold, J.F. Paulson, J. Chem. Phys. 102 (1995) 8865.

[14] W.F. Schneider, T.J. Wallington, J. Phys. Chem. 98 (1994) 7448.

[15] V.I. Vedeneev, V.I. Propoi, O.M. Sarkisov, Kinet. Catal. (Engl. Transl.) 21 (1980) 854.

[16] J.T. Herron, J. Phys. Chem. Ref. Data 16 (1987) 1.

[17] T. Su, W.J. Chesnavich, J. Chem. Phys. 76 (1982) 5183.

[18] M.S. Malmberg, A.A. Maryott, J. Chem. Phys. 53 (1970) 1614.

[19] T.M. Miller, in: D.R. Lide (Ed.), CRC Handbook of Chemistry and Physics, CRC Press, Boca Raton, FL, 1997.

[20] Y. Ikezoe, S. Matsuoka, M. Takebe, A.A. Viggiano, Gas Phase Ion–Molecule Reaction Rate Constants Through 1986, Maruzen Company Ltd., Tokyo, 1987.

[21] W. Sailer, H. Drexel, A. Pelc, V. Gill, N.J. Mason, E. Illenberger, J.D. Skalny, T. Mikoviny, P. Scheier, T.D. Mark, Chem. Phys. Lett. 351 (2002) 71.

[22] R.A. Morris, J. Chem. Phys. 97 (1992) 2372.

[23] J.W. Larson, T.B. McMahon, J. Am. Chem. Soc. 105 (1983) 2944.