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ScienceDirect
Journal of Hazardous Materials 149 (2007) 747–751
Journal of Hazardous Materials
www.elsevier.com/locate/jhazmat

Short communication

The prediction of environmental fate for trifluoromethyl sulfur pentafluoride (SF_5CF_3), a potent greenhouse gas

Wen-Tien Tsai *

Graduate Institute of Bioresources, National Pingtung University of Science and Technology, Pingtung 912, Taiwan

Received 20 June 2007; received in revised form 12 August 2007; accepted 13 August 2007
Available online 19 August 2007

Abstract

Trifluoromethyl sulfur pentafluoride (SF_5CF_3), which is a newly discovered compound in the troposphere and chemically similar to SF_6, has been listed as a potent greenhouse gas because of its high global warming potential close to 20,000 and its long lifetime of about 800 years in the atmosphere. From the environmental and ecological points of view, it is urgent to understand the environmental fate of this unique material, including octanol–water partition coefficient (K_{ow}), water solubility (S) and Henry's law constant (K_H). This article aimed at introducing the greenhouse gas with strong radiative force in its physiochemical properties and potential uses, and predicting its environmental fate on the basis of available methods. The predicted value of log K_{ow}, which was obtained to be about 2.42 at 298.15 K, revealed that it tends to be hydrophobic and partitioned into organic matter, or lipids (fatty tissue). From the predicted values of S and K_H, it was further showed that SF_5CF_3 has exceptionally low solubility in water and extremely high vaporization from the water bodies. These predicted distribution properties have led to the suggestion that it will sink into the atmosphere if it is released into the environment.

Keywords: Trifluoromethyl sulfur pentafluoride; Partition coefficient; Prediction; Environmental fate

1. Introduction

In 1999, Sturges et al. first identified a highly radiative-forcing compound, trifluoromethyl sulfur pentafluoride (SF_5CF_3, CAS No.: 373-80-8), in the atmosphere [1]. The potential original sources of the potent greenhouse gas are probably from the reaction of SF_6 with fluorocarbon under discharge [2], a by-product of fluorochemical manufacturing [3,4], and the recombination of SF_5 and CF_3 radicals on aerosol particles in the terrestrial environment [5]. Such systems likely provide a source of trifluoromethyl groups (CF_3–) from hydrofluorocarbons (e.g., CH_2F_2 and CHF_3), perfluorocarbons (e.g., CF_4 and C_2F_6), or fluoropolymers, which may be further attacked by SF_5 radicals formed in the high-voltage discharge environment containing SF_6. From the data on the infrared absorption spectrum of SF_5CF_3 at 296 K [6], there are five integrated absorption cross-sections observed in the spectral bands of 400–450, 520–640, 670–780, 840–960, and 1125–1325 cm^{-1}, implying that the greenhouse gas possesses the strongest radiative force (0.59 $W\,m^{-2}\,ppbv^{-1}$) on a basis of molecule. Because of its long atmospheric lifetime of approximately 800 years [7,8], it is expected not to be degraded in the tropospheric environment by reactions with hydroxyl radicals once it is emitted into the atmosphere [9].

It should be noted that the concentrations of SF_6 and SF_5CF_3 in the atmosphere have increased over the past decades with a parallel trend each other [1], revealing that the source of SF_5CF_3 may be related to the production of SF_6 and its industrial uses (e.g., gas insulated switchgear) [10]. On the other hand, the atmospheric concentration of SF_5CF_3 increased to about 0.12 ppt in 1999, and is growing at annual rate of 6% $year^{-1}$ [1]. Assuming a constant ratio of SF_6/SF_5CF_3 of 32 [1], the atmospheric concentration of SF_5CF_3 would be about 0.18 ppt in 2006. Based on its atmospheric concentration, the accumulative amount of SF_5CF_3 in the atmosphere currently seemed to be so small that the contribution of this greenhouse gas to global warming is rather small; nevertheless its impacts on the global climate change would be more significant in the future because of its fast growth rate and the relatively high global warming potentials (GWP)-100 year time horizon relative to CO_2 (i.e., 17,500) [8].

* Tel.: +886 8 7703202x7399; fax: +886 8 7740134.
E-mail address: wttsai@mail.npust.edu.tw.

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doi:10.1016/j.jhazmat.2007.08.035

From the viewpoints of molecular structures, SF_5CF_3, chemically similar to SF_6, consists of five fluorine atoms and one CF_3 group attached to a central sulfur atom. The chemical inertness of the octahedral molecule may be due to the fluorine shielding of the sulfur atom. As compared to SF_6, it is a relatively polar compound, indicating that SF_5CF_3 will have a greater affinity for organic matter than SF_6. In order to strengthen our understanding of such fluorinated gas, it is vital to investigate the environmental fate and transport between interfaces like air, water, and solid phases for SF_5CF_3. However, the measured properties regarding the chemical distribution among phases are very scarce in the literature [3,11]. This paper aimed to present the known chemical and physical properties, potentially commercial/industrial uses, and the preliminary predications of octanol–water partition coefficient, water solubility, and Henry's law constant for SF_5CF_3. Furthermore, its environmental fate was discussed in comparison with the fluorinated gas SF_6.

2. The known chemical and physical properties of SF_5CF_3

From the viewpoints of molecular structures, SF_5CF_3 is chemically similar to SF_6. Because of its very low mixing ratio in the atmosphere, its chemical stability and its non-flammability, it has very high potential for use as a refrigerant, tracer gas and electrical insulating gas described in the next section. It is relatively polar as compared to SF_6, implying that SF_5CF_3 will have a greater affinity for organic matter than SF_6.

According to the results by Silvey and Cady [3], SF_5CF_3 could be prepared by the electrochemical process from the reaction of sulfide (e.g., carbon disulfide and methyl mercaptan) with fluoride (e.g., cobalt trifluoride) at 473–523 K. They also obtained the data on the boiling point (252.75 K) and melting point (186.25 K) of SF_5CF_3. Furthermore, the chemical information on this gaseous compound was briefly summarized as follows [3,12]:

1. It is chemically stable because there is no hydrolysis observed in the reaction of the gas with 6 mol/L sodium hydroxide for 2.5 months at room temperature, only reactive with alkali metals at dull red heat, and readily decomposed by spark-over discharge into CF_4 and SF_4 [3].
2. Thermally inert from the pyrolysis experiments, it was heated at 723 K without decomposition in a closed system. However, its reaction with perfluoropropylene (C_3F_6) occurred at temperatures of 698 and 791 K in a nickel-packed reactor, yielding a series of fluorocarbons products including C_2F_6, SF_4, C_4F_{10}, C_5F_{12}, C_6F_{14}, and C_7F_{16} [12].

It is well known that the vapor–liquid behavior of pure component can be described in terms of critical properties such as critical temperature (T_c), critical pressure (P_c), critical density (ρ_c) or critical volume (V_c) because they are used in many corresponding state correlations with thermodynamic or physicochemical properties for a given compound like boiling point (T_b), heat of vaporization (ΔH_{vap}) and vapor pressure (P, kPa) versus temperature (T, K) or reduced temperature (T_r) [13]. With respect to the critical properties and other physicochemical properties of SF_5CF_3 like vapor pressure and dipole moment (μ, D), the information was obtained from the literatures [12,14], and given below:

$T_c = 381.25\,\text{K}$,

$P_c = 3371\,\text{kPa}$,

$\rho_c = 690\text{kg/m}^3$ (or $V_c = 284\,\text{cm}^3/\text{mol}$),

$T_b = 252.85\,\text{K}$,

$\Delta H_{vap} = 20.18\,\text{kJ/mol}$,

$\ln P = 158.745 - 22.1236 \ln T - 8021.2/T$ (Note : $T < T_b$), and

$$\ln P = 16.3152 - 8.3712/T_r - 2.3649 \ln T_r + 0.1790\, T_r^6 \quad (\text{Note} : T_b < T < T_c),$$

$\mu = 0.38\, D(298.15\,\text{K})$

In addition to the critical properties of pure substance, the acentric factor (ω) is commonly used to predict the physical properties. As a reliable approximation, the property, which is related to T_b, P_c, and T_c, was calculated by the following equation [13]:

$$\omega = -[\ln\left(\frac{P_c}{1.01325}\right) + f^{(0)}(T_{br})]/f^{(1)}(T_{br}) \quad (1)$$

where P_c is in bars while T_b and T_c are both absolute temperatures, and T_{br} is defined as the ratio of boiling point (T_b) to critical temperature (T_c). The functions $f^{(0)}$ and $f^{(1)}$ have been defined and given in the references [15,16]. The value of ω of SF_5CF_3 was estimated to be 0.272, close to that (i.e., 0.277) of SF_6 [13], implying that the chemical and physical properties of SF_5CF_3 are very similar to those of SF_6.

3. Potentially commercial/industrial uses of SF_5CF_3

Like SF_6, SF_5CF_3 is a colorless, odorless, tasteless, and incombustible gas at normal conditions. It has very low mixing ratio in the atmosphere due to its high molecular weight (i.e., 196), and it also possesses the highly chemical stability and excellent electrical characteristics because of the six atoms/groups shielding of the sulfur atom. Therefore, its potentially commercial and industrial uses such as refrigerant, tracer gas and electrical insulating gas were further described as follows.

3.1. Refrigerant

Prior to 1990, the majority of domestic refrigerators, freezers and air conditioners used CFC-12 (R-12) and CFC-11 (R-11) as the working fluids due to their thermodynamic properties, chemical stability, non-flammability and non-toxicity. With the

recognition that the productions of hydrochlorofluorocarbons (HCFCs) as interim replacements for CFCs will be totally banned under the treaty of Montreal Protocol, numerous investigations aimed to develop chemicals which can be alternatives to HCFCs for the purpose of protecting the stratosphere ozone layer, including hydrofluorocarbons (HFCs), perfluorocarbons (PFCs), hydrofluoroethers (HFEs), and fluorinated hexavalent sulfur derivatives [13]. For example, the sulfur compounds, CF_3SCF_3 and CF_3SF_5, have been identified during the investigation on their potential as R-12 and R-22 alternatives as either pure chemicals or components of mixtures because they are expected to have a higher solvating power for hydrocarbons than highly fluorinated hydrocarbons. However, it is again emphasized that a significant consideration in using sulfur compounds is that they will be targeted as greenhouse gases (GHGs) in the future, just like SF_6.

3.2. Tracer gas

Because of its very large electron capture cross-section and the possible detection of this gas below parts per trillion (ppt), SF_6 has been commonly used as a tracer gas in the fields of ventilation efficiency in buildings and indoor enclosures, environmental quality modeling in the atmospheric air, ocean, and groundwater [17–19]. It will be expected that SF_5CF_3 has high potential for use in tracer release experiments because it is chemically similar to SF_6.

3.3. Insulating gas

It was well known that gaseous fluorocarbons were specifically useful in high voltage applications as insulating gas for electrical use because of their inert character and high dielectric strength [20]. From the above discussion, CF_3SF_5 was tentatively used as replacement gas for SF_6 as gaseous insulator [21,22], which may be possibly applied to high-voltage circuit breaker, switchgear, substations, transformers, capacitors, transmission lines and other electronic/electrical equipments.

3.4. Other applications

Because of its unique properties under normal conditions, CF_3SF_5 can be potentially of a lot of application, such as fire extinguishing agent, contrast agents in a variety of diagnostic imaging techniques (e.g., ultrasound image), and blowing agent according to the survey from the SciFinder Scholar database.

4. Prediction of properties relating to the environmental fate

In the discussion of environmental distribution among phases for a given compound, it is hypothetical that the target is not chemically transformed. In this respect, SF_5CF_3, chemically similar to SF_6, has been considered to be extremely stable, highly inert and unlikely decomposed under the normal environmental conditions. It means that the environmental fate of the molecule if released or emitted is only transported from a phase to another phase without changing its identities until the equilibrium approached. Therefore, the properties regarding the environmental distribution among air, water, and solid phases are significantly important, not only to understand its movement between media, but also to evaluate its behavior within a single medium. These distribution properties commonly include octanol–water partition coefficient (K_{ow}), water solubility (S), Henry's law constant (K_H), and vapor pressure (P). Recent studies on these properties of SF_5CF_3 measured were only for its vapor pressure [11]. Therefore, the estimation of K_{ow}, S and K_H for SF_5CF_3 based on the chemical's structure was described below. By contrast, the measured or observed data on K_{ow}, S and K_H of SF_6, resembles the chemical structure of SF_5CF_3, at 298.15 K in the literature were also discussed in the work.

4.1. Partition coefficient

Partition coefficient is empirically derived dimensionless property that describes how a chemical substance distributes itself between water phase and oil phase at equilibrium. Hence, it is useful for describing and modeling the environmental fate of an organic compound. Because the octanol–water partition coefficient (K_{ow}) is characterized by partitioning between aqueous and organic, lipid-like phases, it provides a significant indication of how much of an organic compound will be taken up by the fat tissue in aquatic organisms. Because of K_{ow} ranging from 10^{-3} to 10^7, values of K_{ow} are often reported as $\log K_{ow}$ [23]. In general, organic compounds with high values of K_{ow} tend to be hydrophobic and hence partitioned into organic matter, lipids (fat) and soil solid, indicating that they are less mobile in the environment.

It is well known that several methods are available for the estimation of K_{ow} of organic chemicals [23]. However, these approaches are somewhat complicated and not easy to use. The target compound, SF_5CF_3, is a newly synthesized gas containing carbon, sulfur, and fluorine. Thus, there were no measured data on its distribution properties in the literature. In the present paper, the so called Leo's approach [24,25], which is based on the available values of atomic or group fragment constant (f) and structural factor (F), was used for estimating the partition coefficient. For SF_5CF_3, it is feasible to have a measured value of $\log K_{ow}$ for a structurally similar compound (i.e., SF_6); that is,

$$\log K_{ow}(\text{new chemical}) = \log K_{ow}(\text{similar chemical}) \pm \text{fragments}(f) \pm \text{factors}(F) \quad (2)$$

Therefore,

$$\log K_{ow}(SF_5CF_3) = \log K_{ow}(SF_6) - f(-F) + f(-CF_3) \quad (3)$$

The measured or observed value of $\log K_{ow}$ for SF_6 is 1.68 [26]. Based on the limited data on fragment constants [23], the values of fragment attached to aromatic ring have been inevitably used to preliminarily estimate the value of $\log K_{ow}$ for SF_5CF_3; that is,

$$\log K_{ow}(SF_5CF_3) = 1.68 - 0.37 + 1.11 = 2.42$$

In the estimation, it can be seen that the value of $\log K_{ow}$ obtained from the Leo's approach is larger than that of SF_6, indicating that SF_5CF_3 will have a greater affinity for organic matter than SF_6 as expected from their chemical structures. On the basis of their Ostwald coefficients in 1-octanol studied by Smethie et al. [27], it showed that the measured data for SF_5CF_3 is about seven times greater than for SF_6, which is roughly equal to the ratio of the predicted value (i.e., 2.42) for the former to the observed value (i.e., 1.68) for the later. From the predicted value, it can be summarized that the value of partition coefficient for SF_5CF_3 with low-moderate value of $\log K_{ow}$ tends to be hydrophobic and partitioned into organic matter, lipids (fatty tissue), and also have low potential bioaccumulation in the environment [28]. Further, the organic carbon normalized partition coefficient (K_{oc}) for SF_5CF_3 can be possibly predicted from its octanol/water partition coefficient (K_{ow}) by using available relationships [23]. Of course, it would be helpful in measuring K_{ow} in the laboratory to validate the accuracy of the method in the estimation of partition coefficients for SF_5CF_3.

4.2. Water solubility

Of the various fate and transport properties that affect the environmental distribution between air and water, water solubility is one of the most important parameters. However, it is much less important for gases, as compared to liquids or solids, on an environmental basis because it is usually measured when the partial pressure of the gas above the aqueous solution is 1 atm, an unlikely condition in the environment. Henry's law constant (discussed later), another distribution property for gases, is a more important parameter, which describes the ratio of the concentrations of a given gas in the phases of water and air (at low partial pressure) under equilibrium conditions.

Because the octanol/water partition coefficient (K_{ow}) is related to the solubility of a chemical in water (denoted as S), there are different regression equations (i.e., $\log S = a \log K_{ow} + b$) for the estimation of water solubility in the literature [23]. It showed that a plot of $\log S$ versus $\log K_{ow}$ has a slope of about -1 (i.e., $a = -1$). For example, a slope of -0.962 has been correlated with halogenated 1- and 2- carbon hydrocarbons. By using the data on the water solubility of SF_6 in 298.15 K (i.e., 2.47×10^{-4} mol/L, or 4.44×10^{-6} in mole fraction) [29,30], the water solubility of SF_5CF_3 can be roughly estimated to be approximately 4.5×10^{-5} mol/L or 8.1×10^{-7} in mole fraction by using their observed and predicted $\log K_{ow}$ values (i.e., 1.68 and 2.42) for SF_6 and SF_5CF_3, respectively.

4.3. Henry's law constant

Interface transfer between the gas phase (i.e., atmospheric air) and water bodies is one of the fate processes affecting the transport of many chemical compounds in the environment because their vaporization from aqueous solutions is an important pathway from water to air. In this regard, Henry's law is used to describe the partition of a gas in two different phases, such as water and air, under equilibrium conditions. Therefore, the Henry's law constant (K_H) is a partition coefficient, which is usually defined as the ratio of a chemical's concentration in air to its concentration in water at equilibrium, or mathematically described as [13]

$$\lim \left(\frac{f_2}{x_2} \right) x_2 \to 0 = K_H \tag{4}$$

where x_2 is the mole fraction of the solute gas in aqueous solution and f_2 is the fugacity of the solute gas. For dilute solution at low pressure, Eq. (4) is then written as:

$$K_H = \frac{P_2}{x_2} \tag{5}$$

where P_2 is the partial pressure of the solute gas over the solution. In the paper, P_2 is expressed in atmospheres (Pa) and x_2 as a mole fraction, K_H has units of Pa.

For very stable gases, K_H can be proximately estimated by dividing the vapor pressure of a target gas by its water solubility at the same temperature (e.g., 298.15 K) if it has not yet been measured or observed in the literature [23]. The predicted value of $\ln K_H$ (MPa) for SF_5CF_3 was thus obtained to be about 13.3 based on its vapor pressure (i.e., 511 kPa at 298.15 K) [11] and the predicted solubility in water described above. The predicted value implied that the vaporization of SF_5CF_3 from the water bodies to the atmosphere is remarkably high. On the other hand, the predicted value of K_H for SF_5CF_3 is significantly larger than the measured value (i.e., $\ln K_H$ (MPa) = 10.04) of K_H for SF_6 at 298.15 K [31,32]. It was also noted that SF_5CF_3 is very stable in the atmosphere, implying that it does not exactly react with highly oxidative species (e.g., O_3) and free radicals such as hydroxyl radical and could not be decomposed by direct or sensitized photolysis, either. Therefore, this potent greenhouse gas will accumulate in the troposphere and even in the stratosphere.

5. Conclusions

The potential industrial/commercial uses (incl. refrigerant, tracer gas and electrical insulating gas) of trifluoromethyl sulfur pentafluoride (SF_5CF_3), one of the strongest radiative-forcing greenhouse gases on a basis per molecule, has been submitted based on its chemical similarity to sulfur hexafluoride (SF_6). Using the Leo's approach, the octanol–water partition coefficient ($\log K_{ow}$) of SF_5CF_3 has been predicted to be about 2.42 at 298.15 K, revealing that it tends to be hydrophobic and partitioned into organic matter, lipids (fatty tissue) in the environment. According to the predicted values of water solubility and Henry's law constant at 298.15 K, it was further showed that SF_5CF_3 has very low water solubility and extremely high vaporization from the water bodies, suggesting that it will sink into the atmosphere if released into the environment because it does not exactly react with highly oxidative species and free radicals in the troposphere and is also unlikely to biodegrade in the aqueous biosphere.

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