Available online at www.sciencedirect.com
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.

0304-3894/$ – see front matter © 2007 Elsevier B.V. All rights reserved.
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