VAPOR PRESSURE

TEST SUBSTANCE

Identity: Perfluorooctanoic acid, ammonium salt; may also be referred to as PFOA ammonium salt, Ammonium perfluorooctanoate, FC-116, FC-126, FC-169, or FC-143. (Octanoic acid, pentadecafluoro-, ammonium salt, CAS # 3825-26-1)

Remarks: The 3M production lot number was not noted. The test sample is FC-143. Its purity was not sufficiently characterized, though current information indicates it is a mixture of 96.5 - 100% test substance and 0 – 3.5% C_6, C_7, and C_9 perfluoro analogue compounds.

METHOD

Method: Internal. Details outlined under RESULTS section
GLP (Y/N): No
Year completed: 1993

Remarks: As described below, there are a number of methodological concerns with this study. In addition, the document submitted is a combination of two reports. The first report contained Parts I and II, and a second report contained Experiment #3. In addition the first report contains portions of two versions. As neither of the first report versions is dated, it is unknown which is the final version.

RESULTS

Part I: Analysis before and after passing 280 liters of air through various stock solutions.

Procedure: A mixture of 10 ppm FC-95 (PFOS) and 10 ppm FC-143 (PFOA) was prepared in water or water/isopropanol solutions of the polar-organic compounds listed in the table below. Aliquots of each solution were analyzed in triplicate for fluorochemical content by LC-thermospray mass spectrometry both before and after bubbling 280 liters of air through them. The flow rate of the air passing through the stock solutions was 1 L/min. The solutions were kept in an ice bath during bubbling. The concentrations before and after bubbling were compared after adjusting for volume lost during bubbling.

Results

Solution	Original PFOA Conc., ppm	% PFOA retained
500 ppm Tetrabutylammonium	10.0	83
500 ppm Ammonium acetate	10.0	90
503 ppm Laurylpyridinium chloride	10.0	90
500 ppm N-Alkyldimethylbenzylammonium chloride	10.0	101
500 ppm Cetyltrimethylammonium bromide	10.0	95
505 ppm Tallowtrimethylammonium chloride	10.0	90
500 ppm Dicocodimethylammonium chloride	10.0	89
Water/1-Propanol (50:50)	10.0	85
Water/1-Propanol (50:50)	0	0
500 ppm Ammonium acetate in water/1-propanol (50:50)	0.10	98
500 ppm Ammonium acetate in water/1-propanol (50:50)	0.20	108
500 ppm Ammonium acetate in water/1-propanol (50:50)	0.40	85
500 ppm Ammonium acetate in water / 1-propanol (50:50)	0.80	89
500 ppm Ammonium acetate in water / 1-propanol (50:50)	2.00	92

Remarks: These findings appear to suggest a small loss of PFOA. However, in comments dated 12/7/93, Dr. Edwin Tucker of the Chemistry Department at the University of Oklahoma indicates that it is very unlikely that these fluorochemicals were removed by bubbling air through water due to their vapor pressures, which are very low. Tucker thought more likely mechanisms for loss from the solution phase were concentration of the surfactants in foam and loss from the bubbled solutions as foam or micro-droplets.

Part II: Analysis of impinger ammonium acetate solutions.

Procedure: Air was passed through an apparatus containing dry test material and then through glass wool at room temperature to a chain of impingers. A 50:50 propanol:water solution containing 500 ppm ammonium acetate was used in the impingers to catch any volatilized test material. All impingers were in ice water.

Results: No test material was found to be present in either the first or second impinger. This indicates that any test material transported from the solids to air and then into the ammonium acetate solutions in the

impingers is below the detection limit. The calculated maximum vapor pressure was
1.1×10^{-7} torr.

Remarks: In the report, the “maximum” vapor pressure calculated was inadvertently called “minimum” vapor pressure in the text below both equations 5 and 7.

Dr. Tucker stated that the experimental conditions do not provide firm evidence that the number is reasonable. There is no evidence that vapor equilibrium was attained between the solid and the flowing gas.

Experiment #3: Measuring vapor pressure at 90°C

Procedure: The same study as in Part II was conducted in duplicate at 90°C.

Results: The report concludes that PFOA has a measurable vapor pressure at this temperature. The minimum vapor pressure for the test material was purported to be 1.1×10^{-5} torr at 90°C. It was considered a minimum because the impinger trains may not have caught all of the fluorochemical that had been volatilized.

Remarks: There are reasons to consider this a questionable conclusion. The loss of PFOA to the gas phase at 90°C is likely not due to sublimation of the test material. As with any salt, test material would be expected to have a very low vapor pressure. Thus, the minimum "vapor pressure" calculated at 90°C is likely due to decomposition of the test material to NH_3 and the undissociated perfluorooctanoic acid, which is then followed by sublimation of the undissociated perfluorooctanoic acid. This is a well-known mechanism for ammonium salts of organic acids. (1) It is likely to occur at 90°C but not likely to occur at room temperature which is consistent with the observations in this study.

As this volatilization is more likely a sublimation of the acid, not of the test material, one can not make predictions of other physical chemical properties, including the vapor pressure at ambient temperature or Henry’s law constant of PFOA from the value determined in this study.

In addition, the concentrations of the test material in the impinger chain were variable and did not decrease in each sequential impinger. As such a concentration distribution is improbable, this is an indication of possible analytical problems.

CONCLUSIONS

No reliable conclusions can be made based on this study. The general observation is that this compound has very low volatility or a very low vapor pressure under ambient conditions.

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DATA QUALITY

Reliability: Klimisch ranking 3. There is no information on the validity of the analytical method. There is no information on the validity of the test method for determining volatility of the test substance. This study lacks characterization of the purity of the test substance.

REFERENCES

(1) **Recovery of petroleum-derived acids and regeneration of ammonia from aqueous solutions of ammonium salts of petroleum acids.** Abdullaev, R. Kh.; Murshudli, Ch. D.; Shakhmamedova, Z. M.; Kasum-Zade, A. Yu. Azerb. Inst. Nefti Khim., Baku, USSR. Izv. Vyssh. Uchebn. Zaved., Neft Gaz (1987), 30(1), 53-7. CODEN: IVUNA2 ISSN: 0445-0108. Journal written in Russian. CAN 106:216648 AN 1987:216648 CAPLUS

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OTHER

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