STABILITY IN THE ATMOSPHERE (PHOTOLYSIS)

TEST SUBSTANCE

Identity: Perfluorooctanesulfonyl fluoride. May also be referred to as: POSF or FX-8. (1-Octanesulfonyl fluoride, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-) CAS: #307-35-7. Purity: 98%.

Remarks: The Aldrich chemical lot number is 12517LR; test substance is a clear liquid at 25°C.

METHOD

References:

T.J. Wallington et al, *J. Chem. Phys. A* 101, pp. 8264-8274 (1997), and references therein; W.B. DeMore et al, NASA Jet Propulsion Laboratory, JPL Publication No. 94-26 (1994); M.J. Molina et al, "Atmospheric Lifetime Studies of Some Halogenated Ethers (L-14055, L-14056, and L-14093)," report to the 3M Specialty Chemicals Division (March 1996); R.G. Prinn et al, *Science* 269, pp. 187-192 (1995). 3M developed the equipment and analytical techniques required to perform the study.

GLP (Y/N): No, but many GLP procedures followed.
Year completed: 2001
Type: Indirect Gas Phase Photolysis

Test sample preparation: Gaseous reagents POSF, CH_3Cl (at ppm levels), O_3, and H_2O (at percent levels) were added to an evacuated reaction chamber/infrared absorption cell, with balance O_2/He (40%/60%), to one atmosphere. O_3 was generated by illuminating the 40%/60% O_2/He gas mixture with a short-wavelength UV source in a separate reaction chamber and transferring the resulting gas, which contained approximately 1% O_3, to the reaction chamber. Samples were independently prepared immediately before the performance of two sample runs and five control runs.

Analytical Procedures: FTIR techniques were employed to determine the sample concentrations of POSF, CH_3Cl, and O_3 about once per minute; the wavenumber regions employed were 1101.6 – 1320.7, 2824.5 – 3012.7, and 2052.5 – 2141.7 cm^{-1}. Data were collected for approximately 120 minutes per analytical run. For the last ~60 minutes of each run, the mixture was illuminated with 300 to 600 Watts of UV radiation from a broad-band discharge lamp through a window of polished, semi-conductor-grade quartz. The filtered UV radiation generated the gas-phase hydroxyl radical (OH•) - but no additional O_3 - in the reaction chamber. Least-squares analyses of the concentration data yielded six first-order rate constants describing the degradation of POSF, CH_3Cl, and O_3 due to interactions with both OH• and the chamber walls.

RESULTS

Degradation and breakdown products: Indirect photolysis of POSF was not observed in six of the seven sample and control runs. In one control run, with elevated CH_3Cl concentration, some degradation of POSF was observed in the presence of UV radiation and OH•. Comparison of the POSF degradation rate to the published rate constant of the reference CH_3Cl, for this single run, leads to a POSF indirect photolysis half-life of 3.7 years under typical tropospheric conditions.

CONCLUSIONS

The study data generally indicate that reactions between POSF and the OH radical do not occur in the Earth's atmosphere. However, in one run out of seven, a run in which the reference compound monochloromethane (CH_3Cl) was evaluated, we observed a slight decrease in the POSF concentration. The relative rates of degradation of POSF and CH_3Cl observed in this single run are consistent with a POSF half-life of 3.7 years in the presence of typical tropospheric concentrations of the OH radical. Given the lack of degradation in the other six runs, however, it is likely that the actual atmospheric POSF half-life is potentially much longer, than 3.7 years.

SUBMITTEE

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DATA QUALITY

Reliability: Klimisch ranking: 2
Remarks: Study was well conducted, though not under GLP.

REFERENCES

This study was conducted at the 3M Environmental Laboratory under Lab Request Number E01-0739. See 3M Laboratory Report No. E01-0739 (dated 12 June 2001)

OTHER

Last Changed: June 22, 2001