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16. Abstract (Limit: 200 words) The gas phase reaction of N,O-bis-(trimethylsilyl)trifluoroacetamide (BSTFA) with polar organics was validated. Quantitative yields were obtained for alcohols, glycols, glycol ethers and amines using the gas phase derivatization method. These values were then compared with the expected yields from vapor pressure tables. For the formation of methylene-glycol from the reaction of formaldehyde (50000) with water, equilibrium constants were estimated at temperatures ranging from 20 to 40 degrees-C. Gas streams of formaldehyde in air were produced by a gas phase monomeric formaldehyde generator based on acid catalyzed depolymerization of s-trioxane. The formaldehyde was subsequently reacted with water vapor in the air. The chromotropic-acid method was used to determine the concentration of formaldehyde equivalents and BSTFA derivatization method to determine the concentration of methylene-glycol. Temperature dependency of the equilibrium constant is graphed.

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F I N A L R E P O R T

TITLE:

Formaldehyde Molecular States in the Gas Phase

GRANT NUMBER:

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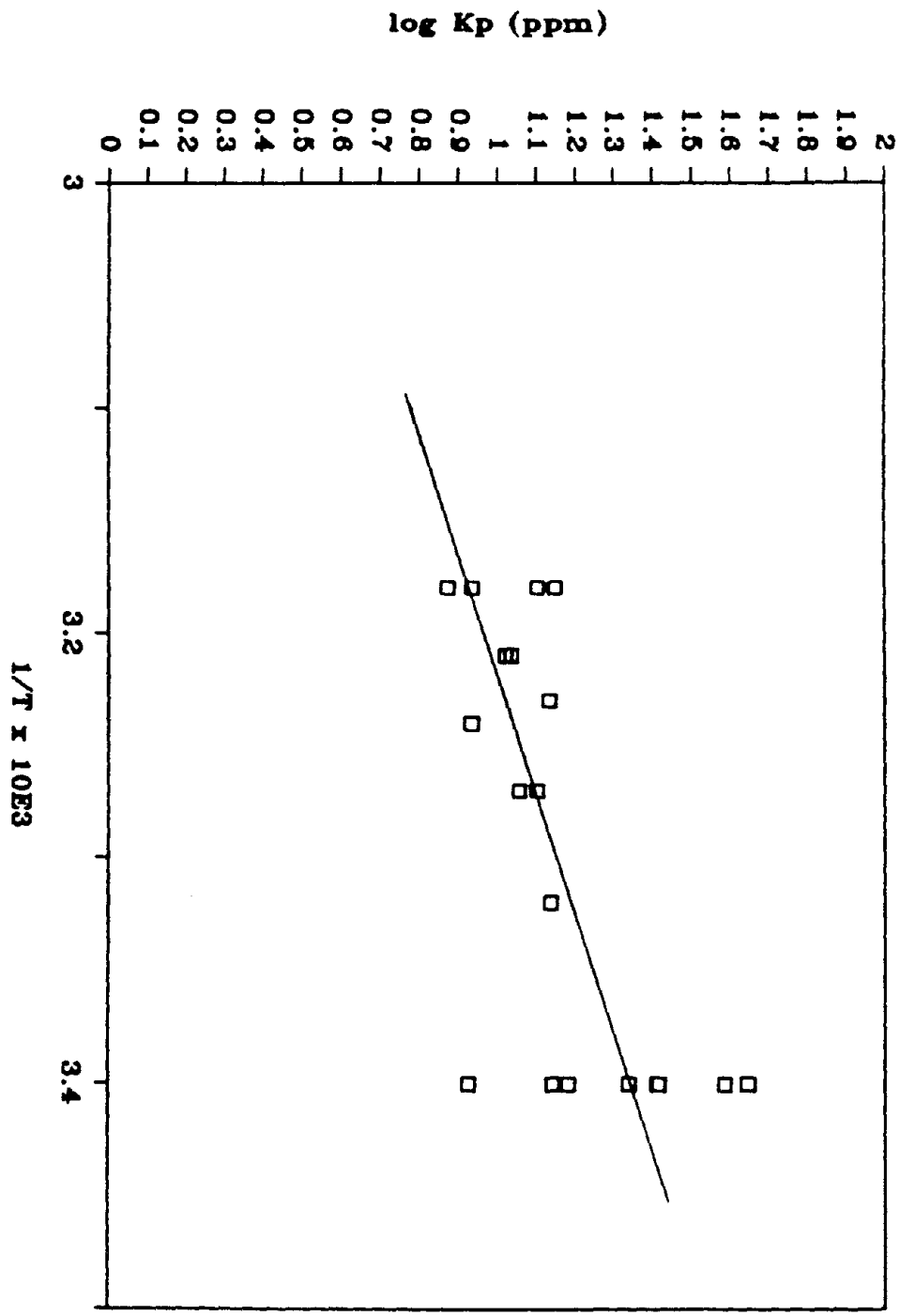
SIGNIFICANT ACHIEVEMENTS:

Validation of the gas phase reaction of N,O-bis-(trimethylsily)trifluoroacetamide (BSTFA) with polar organics was completed. An array of compounds including alcohols, glycols, glycol ethers and amines were analyzed for quantitative yield using the gas phase derivatization method and compared with expected values from vapor pressure tables. Yields are listed in Table I and represent the results of measurements obtained from a replication of the method performed independently by a research associate in our laboratory. The values of % V and % L indicate the relative amounts of the total derivatized product in the vapor and liquid phases in the reaction flasks. In addition to the compounds listed, N-methylaniline and diethylamine were derivatized but could not be resolved from the side-product peaks in the chromatogram.

Equilibrium constants were estimated for the reaction of formaldehyde with water to form methylene glycol in the gas phase over a range of temperatures between 20 and 40°C. A gas phase monomeric formaldehyde generator based on acid catalyzed depolymerzation of s-trioxane was used to produce gas streams of formaldehyde in air that were subsequently reacted with water vapor in air. Aliquots of the reaction mixture were analyzed by (1) chromotropic acid method to determine the concentration of formaldehyde equivalents and (2) BSTFA derivatization method which was used to determine the concentration of methylene glycol. Water vapor concentrations were estimated from vapor pressure data. Temperature dependency of the equilibrium constant is shown in Figure 1.

Table 1. Yields for gas phase derivatization of volatile polar organic compounds using 5:1::BSTFA:DMF solution.

	%V	%L	%Yield	s	N
Methanol	76.5	23.5	87.5	2.9	3
Ethanol	54.6	45.4	91.8	3.3	4
Isopropanol	64.4	35.6	94.9	4.9	4
Phenol	1.4	98.6	68.4	1.1	3
Ethylene Glycol	N.D.	100	69.7	8.9	6
1,3 Butanediol	N.D.	100	111.0	1.5	4
2-Methoxyethanol	12.0	88.0	79.4	13.2	11
2-Ethoxyethanl	8.3	91.7	93.4	11.2	5
Aniline	N.D.	100	92.3	54.1	6


log Kp (ppm)
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0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
1.9
2
3
3.2
3.4
1/T x 10E3

Kp(ppm) vs 1/T