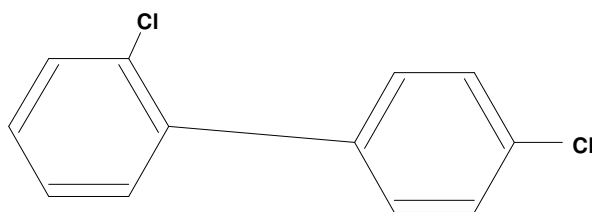


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PIM #1

Estimating the Enthalpy of Vaporization for Semivolatile Industrial Compound, 2,4'-dichlorobiphenyl at Pellston, Michigan

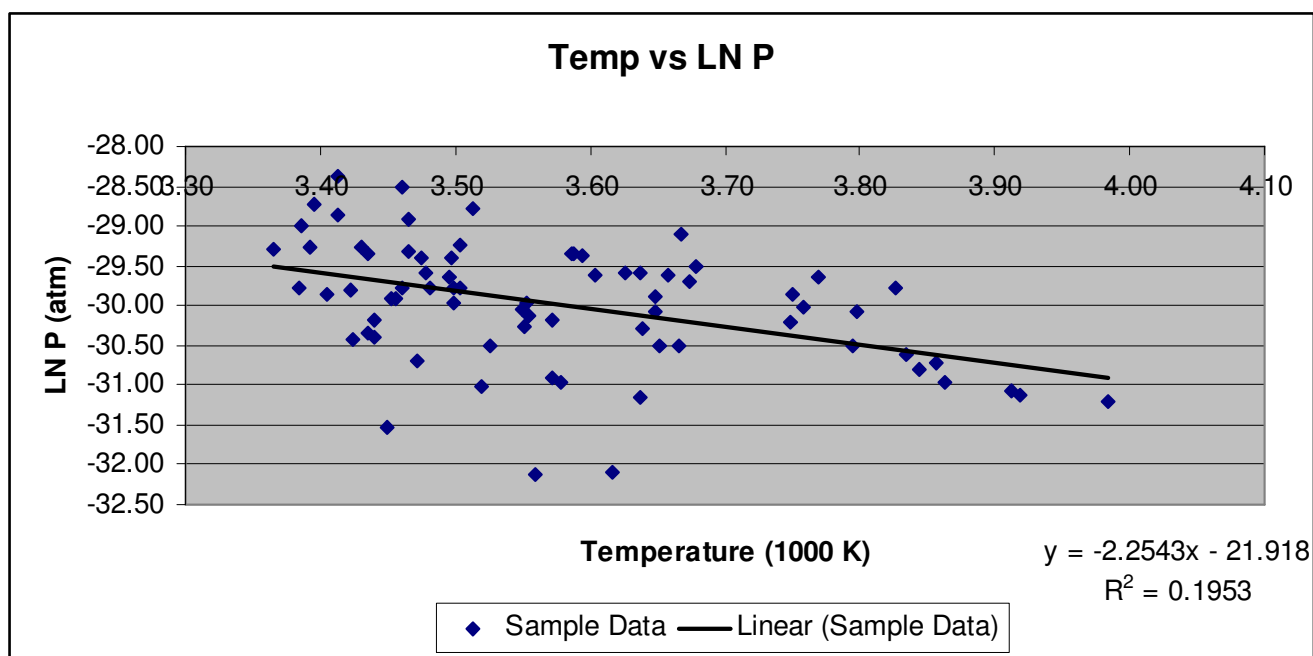
Polychlorinated biphenyls, or PCB's have been used in the produce industry for years as an effective pesticide; however, they have been known to cause damage to people and ecosystems. PCBs have not been in use for many years but the effect has been felt decades later. PCBs are still present in various concentrations. Pelleston, Michigan is the location of data that was collected from May 1992 to February 1994. Samples were collected every six days from Pelleston and concentrations of 2,4'-dichlorobiphenyl were recorded.



2,4'-dichlorobiphenyl

Data

See attached Excel worksheet.



Data Analysis

SUMMARY OUTPUT

<i>Regression Statistics</i>	
Multiple R	0.442111883
R Square	0.195462917
Adjusted R Square	0.184288791
Standard Error	0.693506427
Observations	74

ANOVA					
	<i>df</i>	<i>SS</i>	<i>MS</i>	<i>F</i>	<i>Significance F</i>
Regression	1	8.413017362	8.41301736	17.4924566	8.02345E-05
Residual	72	34.6284838	0.48095116		
Total	73	43.04150116			

	<i>Coefficients</i>	<i>Standard Error</i>	<i>t Stat</i>	<i>P-value</i>
Intercept	-42.9138857	1.988752818	-21.57829	3.7056E-33
AVG TEMP (1/T)	2.96918E-05	7.09922E-06	4.18239843	8.0235E-05

- The regression data analysis indicated that there is not a strong linear relationship because the r value = 0.442
- Since $Significance F = \rho$, and $Significance F < \alpha$, then there is a linear relationship.
- $-\Delta H = R * \text{slope of the regression line}$
 $-\Delta H = (8.314 \text{ J/mol}\cdot\text{K}) * (-2.2543)$
 $\Delta H = 18.74 \text{ kJ/mol}$ (kJ/mol are the units because the factor of 1000 was already taken into account)
- There does not appear to be an indication that 2,4'-dichlorobiphenyl is a local source at Pellston, Michigan. $\Delta H = 18.74 \text{ kJ/mol}$. This low ΔH , would seem to indicate that there would not be a significant local source of 2,4'-dichlorobiphenyl.

Group Data

Figure 1

Summary of Pellston, MI

Group Member	PCB	Compound	ΔH (kJ/mol)	HLC (atm-m ³ /mole)
Justin	8	2,4'-dichlorobiphenyl	18.74	0.00023
Joe	28	2,4,4'-trichlorobiphenyl	20.78	0.0002
Pat	52	2,2',5,5'-tetrachlorobiphenyl	27.37	0.0002
Natalie	118	2,3',4,4',5-pentachlorobiphenyl	25.76	0.000288

- ◆ Highest $\Delta H = 27.37$ kJ/mol
- ◆ Lowest $\Delta H = 18.74$ kJ/mol

Regression Statistics	
Multiple R	0.189356
R Square	0.035856
Adjusted R Square	-0.44622
Standard Error	4.894047
Observations	4

ANOVA					
	df	SS	MS	F	Significance F
Regression	1	1.781478	1.781478	0.074378	0.810644429
Residual	2	47.9034	23.9517		
Total	3	49.68488			

Conclusions

Air sample data for 2,4'-dichlorobiphenyl was collected over a period of two years. ΔH was determined from a plot of temperature vs Ln P. After a regression analysis was performed there appears to be no strong linear relationship between increasing temperature and Ln pressure. The Henry's Law Constant (HLC) is equal to 0.00023 atm-m³/mole at 25 degrees Celsius. Henry's Law Constant is considered to be an indicator on how easily a compound moves to the atmosphere. The constant accounts for the dissolution of the compound into water and air. According to Hermanson, et al, 2007, Henry's Law Constant is a good indicator of pesticide transfer into the gas phase. 2,4'-dichlorobiphenyl has a low HLC, so it does not exist in the atmosphere easily. This conclusion is supported by my low value of ΔH . Compounds with large vapor pressure and low water solubility will move into the atmosphere more readily. 2,4'-dichlorobiphenyl does not appear to do this.

When comparing data from three other chemicals in Pellston, MI, each chemical had a low ΔH value. Also, there appears to be no correlation between ΔH and HLC. Therefore, there is no indication of pollution from a local source and no indication that there are pesticides in the air.

References

Hermanson, Mark H., and D. Moss, C. Monosmith, G. Keeler (2007), Spatial and temporal trends of gas and particle phase atmospheric DDT and metabolites in Michigan: Evidence of long-term persistence and atmospheric emission in a high-DDT-use fruit orchard, *Journal of Geophysical Research*, vol. 112, D04301.