CORRELATING MOLECULAR STRUCTURES AND PROPERTIES OF EMERGING CONTAMINANTS WITH ENVIRONMENTAL FATE MODELS

By

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CHAPTER I

INTORDUCTION

1.1 Emerging Contaminants of Environmental Concern

Pharmaceuticals, antibiotics, hormones, personal care products, nanoparticles, and their degradation products have been observed throughout our ecosystem and in some cases in our drinking water (Borch, et al., 2009). This new category of emerging contaminants has attracted the attentions of citizens, scientists and engineers, researchers, state and federal agencies, environmental groups, industrial and commodity groups, and regulators (Yan, et al., 2010). Emerging contaminants have been associated with significant environmental impacts, for example selected pharmaceuticals have been associated with feminization of fish and the non-steroidal anti-inflammatory drug, diclofenac, has been shown to be responsible for the catastrophic decline in vulture populations in Asia and thus, emerging contaminants present numerous challenges for scientists, engineers, regulators and the public (Kehoe, et al., 2007). There are some 60,000 chemicals in current commercial production with approximately 1000 being added each year, and perhaps 500 substances are of environmental concern because of their presence in detectable quantities in various components of the environment, their toxicity, their tendency to bioaccumulate, or their persistence (Mackay, et al., 1997).

These emerging contaminants and their degradation products pose environmental risk and hence need to be regulated. Thus it is crucial to assess the environmental risks associated with the production, transportation, utilization and disposal of the emerging contaminants. There are very limited or no experimental data available for most of the thousands of organic compounds that are produced and often released into the environment (Reinhard and Drefahl, 1999). New pesticides, pharmaceuticals, personal care products and other chemicals are produced at rates that cannot be matched by experimental attempts to determine the outcome when spilled or released into the environment, making it essential to develop systems that can predict their fate in the environment before experimental assessment (Gomez, et al, 2007).

1.2 Quantitative Structure-Activity Relationships (QSARs)

The assessment of fate and distribution of environmental pollutants in various phases including air, water, and soil is important for the risk assessment of chemicals (Basak, et al., 2007). There is also a considerable interest in developing methods for predicting the properties (e.g. Solubility) and activities (e.g. fate, toxicity) of chemicals, especially organics, in the environment and in engineered systems (Sawyer, et al., 2003). Characteristics of organic compounds (physical, chemical and structural) are used and correlations have been developed for a wide variety of structures, properties, and activities (Sawyer, et al., 2003). Various authors have attempted to model important physicochemical properties using quantitative structure-property relationships (QSPRs) and quantitative structure-activity relationships (QSARs) based on calculated molecular descriptors. The tools and approaches used to generate a QSPR and a QSAR are similar.

Quantitative structure-activity relationships (QSARs) are statistically derived models that can be used to predict the physicochemical and biological (including toxicological) properties of molecules from the knowledge of chemical structure (Roy et al, 2009). The description of QSAR models has been a topic for scientific research for more than 40 years and a topic within the regulatory framework for more than 20 years. QSARs are being applied in many disciplines like drug discovery and lead their optimization, risk assessment and toxicity prediction, regulatory decisions, and agrichemicals. QSARs were initially used in drug design and formulation of pesticides, and later extended for use in environmental toxicity.

In QSAR, structural molecular properties of compounds (called descriptors) are correlated with functions (like physicochemical properties, biological activities, toxicity, etc.) by the means of statistical methods resulting in a simple mathematical relationship as shown in equation 1 below.

Function = f (structural, molecular or fragment properties) Equation (1)

'Calculated structural molecular descriptors are preferred to simple experimental or calculated properties in developing quantitative structure–activity/property relationships (QSAR/QSPR) models to predict the physicochemical, biological or toxicological properties of chemicals for the following reasons

a. More than 50% of the current commercial and industrial chemicals have no available experimental data on physicochemical properties or toxicities, and two to three thousand new chemicals are added to this list every year. Determination of the experimental data for all these chemicals would be a Herculean task involving billions of dollars, the sacrifice on many test animals, and enormous amounts of time.

b. In drug design, properties often have to be predicted for the virtual libraries of compounds that are not yet synthesized.

c. Calculation of the structural molecular descriptors requires no information other than the molecular structure, and their computation is fast.' (Kraker, et al., 2007)

Hammett correlated some electronic properties of organic acids and bases with their equilibrium constants and reactivity (Tang, 2003). This was the most significant development in QSARs. Hansch and Leo (1995) used log P in QSAR methods as a general description of cell permeability. Katritzky et al., (1998) used descriptors calculated by CODESSA (CODESSA Comprehensive Descriptors for Structural and Statistical Analysis), a comprehensive program for developing quantitative structure-activity/property relationships (QSAR/QSPR) by integrating all necessary mathematical and computational tools, in the formulation of QSPRs for a diverse set of 411 chemicals. Engelhardt et al., (2000) used topological descriptors and computational neural networks (CNNs) in the formulation of QSPRs for the estimation of vapor pressure (VP) for a diverse set of 420 organic compounds. Liang and Gallagher (1998), along with Staikova et al., (2004), used quantum chemically derived indices, polarizability in particular, in the development of QSPRs for vapor pressure estimation. Summarizing the objective of QSAR one can say that QSAR models allow us to predict the activities of untested and sometimes yet unavailable compounds, and to provide insight of which relevant and chemical properties are determinant for the activity of compounds.

1.3 Scope of Investigation

In this study an attempt was made to develop correlations between physical chemical properties of geosmin, 2-methylisoborneol, acetaminophen, triclosan, atrazine and 2,4-dichlorphneol with their degradation rate constants. Because of their ubiquitous presence in water and the risk associated with them, geosmin, 2-methylisoborneol, acetaminophen, triclosan, atrazine and 2,4-dichlorphneol- were chosen for this research project to investigate their environmental fate through the use of quantitative structure activity relationships. The physical-chemical properties used as descriptors in this study are: log octanol/water partition coefficient (Log K_{OW}), solubility in water, vapor pressure, Henry's law constant, log octanol/air partition coefficient (Log K_{oa}), soil adsorption coefficient (K_{OC}), enthalpy of vaporization, energy of highest occupied molecular orbital (E_{HOMO}) and energy of lowest unoccupied molecular orbital (E_{LUMO}). These descriptors were correlated with biodegradation rate, oxidation rate and hydrolysis rate constants, which are important properties of compounds in determination of environmental fate. The purpose of this study was to investigate whether physical chemical properties of a compound helps in predicting degradation rate constants. Thus by knowing some of the physical chemical properties of a compound, its fate in environment, risk associated with release of chemicals in the environment and methods to treat the compound when released in the environment can be estimated.

CHAPTER II

REVIEW OF LITERATURE

2.1 **Introduction to Taste and Odor causing compounds (Geosmin and 2-Methylisoborneol)**

Removing taste and odor compounds from drinking water is a significant challenge for water authorities internationally (Cook, et.al, 2000). The majority of all biologically caused taste and odor outbreaks in drinking water characterized worldwide are caused by microbial production of geosmin and 2-methylisoborneol (Juttner and Watson, 2007). These two earthy-muddy-smelling metabolites have been the focus of considerable research since early 1960s, still geosmin and 2-MIB remain poorly understood throughout much of the water industry, and misconceptions which impede the prediction, treatment, and control of these volatile organic compounds (VOCs) persist (Juttner and Watson, 2007). These compounds are primarily formed intracellularly in blue-green algae (cyanobacteria) and actinobacteria, and are released upon cell destruction. Although taste and odor problems are not considered a direct threat to public health, they are of great concern for many water utilities because consumers generally rely on the taste of their water as the primary indicator of its safety. These two compounds can be detected by consumers as a musty-earthy odor at levels as low as 10 ng/L (Cook, et al., 2000). There are currently no regulations for these two compounds as they have not been associated with any health effects (OWWRC, 2008).

The main challenge faced by the utilities in the treatment of geosmin, 2-MIB and other odor causing substances is associated with their extremely low odor threshold concentrations (OTC) (McGuire, 1995).The OTC for geosmin and MIB are 4 ng/L and 9 ng/L, respectively. Therefore, the treatment methods for these compounds must be very effective (Cook, et.al, 2000).

2.2 Causes of Taste and Odor

Taste and odor can enter water in a variety of manners. Surface water sources can become contaminated through algal blooms or through industrial wastes or domestic sewage introducing taste- and odor-causing chemicals into the water (Hou and Clancy, 1997). Groundwater supplies can be afflicted with dissolved minerals, such as iron and manganese, which enter the water when it passes through rocks underground. Tastes and odors can also enter either type of water in the raw water transmission system and in the treatment plant due to algal growths, accumulated debris and sludge, or disinfection byproducts. The distribution system can have many of the same causes of taste and odor mentioned above, with the addition of problems resulting from cross-connections and low flow zones (Hou and Clancy, 1997). In table 1, a summary of various taste and odor causing chemicals is presented.

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Table 1 Lists of chemicals causing taste and odor problems in water (Hou and Clancy, 1997)

Chemical cause	Taste/odor	Origin
Geosmin	earthy or grassy odors	Produced by actinomycetes, blue-green algae, and green algae.
2-Methylisoborneol (MIB)	musty odor	Produced by actinomycetes and blue-green algae.
2t, 4c, 7c-decatrienal	fishy odor	Produced by blue-green algae.
Chlorine	bleach, chlorinous, or medicinal taste and odor	Addition of chlorine as a disinfectant.
Chloramines	swimming pool, bleach, or geranium odor	Addition of chlorine and ammonia as a disinfectant.
Aldehydes	fruity odor	Ozonation of water for disinfection.
Phenols and Chlorophenols	pharmaceutical or medicinal taste	Phenols usually originate in industrial waste. Chlorophenols are formed when phenols react with disinfecting chlorine.
Iron	rusty or metallic taste	Minerals in the ground.
Manganese	rusty or metallic taste	Minerals in the ground.
Hydrogen sulfide	rotten egg odor	Produced by anaerobic microorganisms in surface water or by sulfates in the ground.
Methane gas	garlic taste	Decomposition of organic matter.
Isobutanal	Sweet/fruity or malty-odor	Byproduct from ozonation, chlorination and chloramination

2.3 Sources and Properties of Geosmin and MIB

Taste and odor can originate from algae in source water, result from water treatment processes or develop in distribution systems. Odor compounds may originate from industrial and municipal sewage effluents or from biological activities of algae and heterotrophic microorganisms (Cees, et al., 1974).

In the period of 1967-1970 two earthy smelling metabolites of *Streptomyces* strains and blue-green algae were identified as geosmin and 2-methylisoborneol and their important role in different water odor problems in the U.S.A. was established (Safferman, et al., 1967). The two compounds were originally identified from isolates of aerobic filamentous actinomycete bacteria and these organisms for some time were and often still are perceived by water industry as the major source of these Volatile Organic Carbons (VOCs). The two compounds are principal odor components of soil and periods of high terrestrial runoff may introduce actinomycetes and/or their odorous metabolites into surface waters, causing episodic odor outbreaks in rivers, particularly in areas of intensive livestock operations (Juttner and Watson, 2007).

The structure of geosmin was first established as *trans*-1, 10-dimethyl-*trans*-9-decalol by Gerber (1965) who detected the volatile oil in 17 different species of *Streptomyces* and blue-green algae following its initial isolation from *S. griseus*. Cyanobacteria (blue-green algae), photoautotroph's, were recognized as a more frequent source of geosmin and 2-methlyisoborneol in water than actinomycetes (Krishnani, et al., 2008). Geosmin in treated water drinking water was traced to the disturbance of thick biofilms that had developed on the pipe surface of a distribution system from groundwater-supplied treatment plant (Juttner, unpublished data, quoted in Juttner and Watson, 2007). Cyanobacteria are considered to be the chief sources of geosmin and MIB. Fewer than 50 of the more than 2000 species classified to date (according to International Code of Botanical Nomenclature) have been directly confirmed as producers, while the majority have yet to be investigated for their production of these and other VOCs. Unsightly and highly visible surface blooms are usually considered to be primary sources of source

water odor, but in fact many of the known cyanobacterial producers are non-planktonic (≈ 30%), while the remainder are benthic or epiphytic, with a single isolate from soil (Juttner and Watson, 2007).

The most common causes of taste and odor issues are geosmin and 2-methylisoborneaol (MIB), which are naturally occurring compounds produced by blue-green algae (cyanobacteria), diatoms, and actinomycetes. Geosmin and 2-MIB are tertiary alcohols, each of which exists as (+) and (-) enatiomers. Odor outbreaks are caused by biological production of the naturally occurring (-) enatiomers. The (-) enatimoers are ten times more potent than the (+) molecules (Juttner and Watson, 2007). Geosmin and 2-MIB are produced by members of certain groups of benthic and pelagic aquatic microorganisms found in source waters such as lakes, reservoirs, and running waters. Other biological sources mainly originate from terrestrial ecosystems, industrial waste treatment facilities and drinking water treatment plants.

2.4 Geosmin and 2-MIB producing species

Geber and Lechevalier (1965) isolated geosmin, an earthy-smelling substance in 1964. Geosmin and MIB were first identified in actinomycetes, then later in cyanobacteria and fungi that inhabit aquatic and soil environments (Krishnani, et al., 2005). Tables 2, 3 and 4 present the various species producing MIB, geosmin and both, respectively.

Table 2 2-MIB-producing species (Krishnani, et al., 2005)

Species	Origin	Habitat	References
Oscillatoria			
O. perornata (Planktothrix MS988)	Fish pond/USA	Planktonic	van der Ploeg et al. 1995; Tellez et al. 2001a, b; Taylor et al. 2006
O. limosa	Lake/USA	Benthic	Izaguirre and Taylor 1995
Oscillatoria sp.	Fish pond/USA	Planktonic	Martin et al. 1991
O. tenuis	Japan	Planktonic	Negoro et al. 1988
O. geminata	Fish pond/Japan	Fish Pond	Matsumoto and Tsuchiya, 1988
O. limnetica	Fish pond/Japan	Fish Pond	Matsumoto and Tsuchiya, 1988
Oscillatoria cf. curviceps	Lake/USA	Benthic	Izaguirre et al. 1982, 1983
O. tenuis	Water supply/USA	Benthic	Izaguirre et al. 1983
O. variabilis	Fish farming lake/ Japan	Benthic	Tabachek and Yurakowski 1976
O. chalybea	Reservoir/ Israel	Benthic	Leventer and Eren 1970
Phormidium			
Phormidium LP684	Lake/USA	Benthic	Taylor et al. 2006
Phormidium aff. formosum	Water supply/ Australia	Benthic	Baker et al. 2001
P. favosum	Lake/Japan	Benthic	Sugiura et al. 1997
Phormidium	USA	Benthic	Izaguirre 1992
P. tenue	Lake/Japan	Benthic	Sugiura et al. 1986
P. tenue	Water supply/ Japan	Planktonic	Yagi et al. 1983
Pseudanabaena			
Pseudanabaena	Reservoirs/USA	Planktonic	Izaguirre et al. 1999; Taylor et al. 2006
Pseudanabaena	Lake/USA	Planktonic	Izaguirre and Taylor 1998
Other species			
Synechococcus sp.	Water reservoirs/USA	Planktonic	Taylor et al. 2006
Leptolyngbya sp.	Periphyton, lake/USA		Taylor et al. 2006
Lyngbya LO198	Reservoir/USA	Benthic	Taylor et al. 2006
Hyella	Aqueduct water/USA	Epiphytic	Izaguirre and Taylor 1995
Lyngbya Cal.Aq.892	Aqueduct lake/USA	Epiphytic	Izaguirre and Taylor 1995
Planktothrix MS988	Catfish pond/ USA	Planktonic	Martin et al. 1991

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Species	Origin	Habitat	References
Planktothrix cryptovaginata	Fish, water/Finland	Benthic	Persson 1988
Jaaginema geminatum	River/Japan	Benthic	Tsuchiya and Matsumoto, 1988
Synechococcus sp.	Plankton, lake/USA	Planktonic	Izaguirre et al. 1984
Lyngbya cf. *aestuarii*	Fish farming lake / Japan	Benthic	Yurkowski and Tabachek, 1980; Tabachek and Yurkowski 1976

Table 3 Geosmin-producing species (Krishnani et al. 2005)

Species	Origin	Habitat	References
Anabaena			
Anabaena sp.	Lake/USA	Planktonic	Saadoun et al. 2001
A. laxa CA 783	Lake plankton/USA	Planktonic	Rashash et al. 1996
A. crassa LS698	Lake/USA/Australia	Planktonic	Baker et al. 1994; Komarkova-Legnerova and Cronberg, 1992
A. circinalis	River/Australia	Planktonic	Bowmer et al. 1992
A. circinalis	Reservoir/USA	Planktonic	Rosen et al. 1992
A. solitaria	Taiwan	Planktonic	Wu et al. 1991
A. viguieri	Taiwan	Planktonic	Wu et al. 1991
A. macrospora	River/Japan	Planktonic	Tsuchiya and Matsumoto, 1988
A. scheremetievi	Water supply/USA	Planktonic	Izaguirre et al. 1982
Elenkin			
Oscillatoria			
O. limosa	River/Spain	Benthic	Vilalta et al. 2003, 2004
O. limosa	River/Reservoir/ Netherlands		van Breeman et al. 1992
Oscillatoria sp.	Periphyton, river/ (Philadelphia) USA	Benthic	Burlingame et al. 1986
O. brevis	Inland water/Norway	Benthic	Berglind et. al. 1983b
O. simplicissima	Water supply/USA	Pipeline	Izaguirre et al. 1982

Continued on next page

Species	Origin	Habitat	References
O. tenuis	Fish pond/Israel		Aschner et al. 1967
Phormidium			
Phormidium LS1283	Algae, lake/USA	Benthic	Taylor et al. 2006
Phormidium cf. inundatum LO584	Reservoir/USA	Sediment	Taylor et al. 2006
Phormidium sp. (SDC202a,b,c)	Canal/USA		Taylor et al. 2006
Phormidium sp. DCR301	Reservoir/USA	Sediment	Taylor et al. 2006
Species	Origin	Habitat	References
Phormidium sp. ER0100	Reservoir/USA	Sediment	Taylor et al. 2006
Phormidium DC 699	Algae/lake/USA	Benthic	Taylor et al. 2006
Phormidium sp. LD499	Algae/ lake	Benthic	Taylor et al. 2006
Phormidium sp. LM494	Lake/USA	Sediments	Taylor et al. 2006
Phormidium sp. LS587	Lake/USA	Sediments	Taylor et al. 2006
Phormidium sp. R12	Canal/USA		Taylor et al. 2006
P. allorgei	Lake/Japan	Benthic	Sugiura et al. 1997
Phormidium sp.	Lake/USA	Benthic	Izaguirre and Taylor, 1995
P. amoenum	Japan	Benthic	Tsuchiya and Matsumoto, 1988
P. simplissimum	Fish, water/Finland	Benthic	Persson 1988
P. formosum	Fish, water/Finland	Benthic	Persson 1988
P. cortianum	Fish farming lake/ Japan	Benthic	Tabachek and Yurakowski, 1976
Other geosmin-producing species			
Nostoc sp.	Creek/USA	Periphytic	Taylor et al. 2006
Microcoleus-like cyano	Aqueduct/USA	Epiphytic	Izaguirre and Taylor, 1995
Lyngbya cf. subtilis	Aquaculture pond/ USA	Benthic	Schrader and Blevins, 1993
Planktothrix prolifica	Norway	Benthic	Naes et al. 1988
Aphanizomenon gracile	Lake/Germany	Planktonic	Jüttner 1984

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Species	Origin	Habitat	References
Tychonema bornetii	Lake/Norway	Benthic	Berglind et al. 1983a
Schizothrix muellerii	Japan	Benthic	Kikuchi et al. 1973
Symploca muscorum	Fish farming lake/ Soil Japan		Tabachek and Yurakowski 1976 (first reported by Medsker et al., 1968)
Geitlerenema splendidum	Fish farming lake/ Japan	Benthic	Tabachek and Yurakowski, 1976
Actinomycetes			
Streptomyces halstedii	Aquaculture pond/ USA	Sediments	Schrader and Blevins,2001
Streptomyces griseus	USA		Gerber and Lechevalier 1965

Table 4 Geosmin- and 2-MIB-producing species (Krishnani et al. 2005)

Species	Origin	Habitat	References
Phormidium			
Phormidium sp. Cal Aq.0100	Aqueduct/USA	Periphyton	Taylor et al. 2006
Phormidium sp.HD798	Algae/lake	Periphytic	Taylor et al. 2006
Phormidium sp.	Lake/USA	Benthic	Izaguirre 1992
Phormidium sp.	River/Japan	Benthic	Matsumuto and Tsuchiya 1988
Phormidium sp.	Inland water/ Norway	Benthic	Berglind et al. 1983b
Other species			
Synechococcus sp CL792	Lake/USA	Planktonic	Taylor et al. 2006
Nostoc sp.	Water treatment plant /Taiwan		Hu and Chiang 1996
T. granulatum	Japan	Benthic	Tsuchiya and Matsumoto 1988
Planktothrix agardhii	Lake/Norway	Planktonic	Persson 1988; Berglind et al. 1983a
O. brevis			Berglind et al. 1983b
Actinomycetes			
Streptomyces	Denmark	Streams/pond	Klausen et al. 2005
Streptomyces violaceusniger	Water supply/ Jordon	Sediment	Saadoun et al. 1997
Streptomyces sp.	USA		Gerber 1977

2.5 Substrates for growth of species producing Geosmin and 2-MIB

Zaitlin and Watson (2006) studied how different carbon sources influence the activity and growth of microorganisms in the environment. Schrader and Blevins (2001) evaluated the effect of carbon source, phosphorous and other nutrients on species producing geosmin and MIB. More readily assimilated carbon sources such as glucose were found to increase biomass but not geosmin production (Zaitlin and Watson, 2006). Geosmin per capita and total biomass production increased when phosphorous increased from 0 up to 36 mM while zinc, copper and iron inhibited geosmin production and potassium appeared to have little effect (Zaitlin and Watson, 2006). Copper sulphate addition increased biomass and per capita yield of geosmin in *S. tendae*, while manganese, magnesium, iron, cobalt, nickel and zinc had limited effects on both growth and per capita geosmin production (Dionigi, et al., 1996). Increased atmospheric carbon dioxide levels and whole cells or lysed cells of the cyanobacterium *Oscillatoria tenuis* also increased geosmin production, though not biomass production (Schrader and Blevins, 2001). Geosmin production may also be related to growth stage of the actinomycete. Mutants of *Streptomyces sp*. that lost the ability to produce spores or aerial mycelium also stopped producing geosmin (Redshaw, et al., 1979; Bentley and Meganathan, 1981). Normal isolates grown on medium that was not conducive to sporulation reduced their geosmin biosynthesis compared to those grown on medium that promoted sporulation (Dionigi, et. al., 1992).

2.6 Biosynthesis of Geosmin and 2-MIB

2-MIB is a monoterpene and geosmin is an irregular sesquiterpene. The figure 1 below shows the simplified biosynthetic scheme for the formation of 2-MIB and geosmin in streptomycetes and myxobacteria. The structure of geosmin was first established as *trans*-

1, 10-dimethyl-*trans*-9-decalol by Gerber (1965) who detected the volatile oil in 17 different species of *Streptomyces* and a blue-green alga following its initial isolation from *S. griseus*. Shortly thereafter, Bentley (1981) provided evidence that the C12 metabolite geosmin was likely a degraded sesquiterpene, based on the apparent incorporation of both [1-14C]- and [2-14C]acetate into geosmin by strains of *S. antibioticus*.

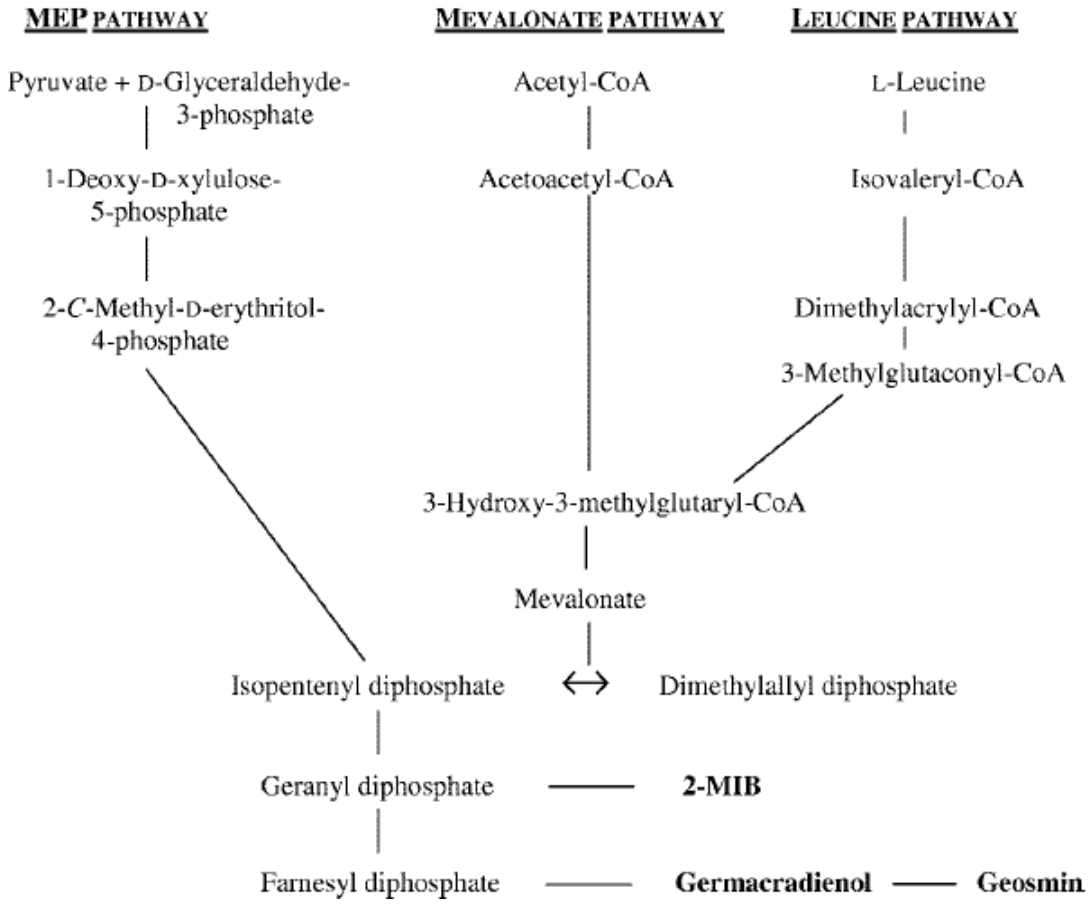


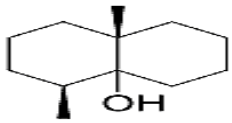
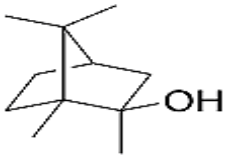
Figure 1 Simplified Biosynthetic scheme for formation of 2-MIB and Geosmin in streptomycetes and myxobacteria (Juttener and Watson, 2007)

2.7 Properties of Geosmin and 2-MIB

2-MIB and geosmin are susceptible to biological degradation (biodegradation) with several studies having implicated a variety of microorganisms responsible for their removal from water. Both cyanobacteria and actinomycetes produce geosmin and 2-methylisoborneol. Geosmin has an earthy odor, which can be defined as dirt, corn silk, and beet while 2-methylisoborneol has a musty odor that can be defined as damp basement (Gerber, 1969), and the properties of these two compounds are summarized in table 5. Geosmin and 2-MIB are produced intracellularly and its release to the water occurs mainly when the algae producing it die and decompose.

Table 5 Properties of Geosmin and 2-MIB (Krishnani et al. 2005)

Property	Geosmin	2-MIB
Chemical Name	*trans*-1,10-Dimethyl-*trans*-9-decalol	1,2,7,7-Tetramethyl-exo-bicyclo-heptan-2-ol
Molecular Formula	$C_{12}H_{22}O$	$C_{11}H_{20}O$
Molecular Weight (g/mol)	182.31	154.25
Molar Volume (cm^3/mol)	231	210
Appearance	Light Yellow Oil	White Solid
Boiling Point (^{0}C)	270	-
Odor Threshold Concentration (ng/L)	6-10	2-20
Henry's Law Constant at 20^0C	0.0023	0.0027

Density at 20^0C (g/ml)	0.949	0.929
Water Solubility at 20^0C (mg/L)	150.2	194.5
Vapor Pressure (atm)	5.49×10^{-5}	7.26×10^{-5}
Enthalpy (kJoule/mole)	82.5 ± 13.3	78.7 ± 9.9
CAS	16423-19-1	2371-42-8
Structure		

2.8 Evaluation of taste and odor problems in drinking water

Taste and odor caused by various chemicals and organisms in source water and in distribution system have been identified (Suffet, et al., 2004). The combined use of highly sophisticated analytical techniques such as gas chromatography/mass spectrometry and sensory panel techniques have made it possible to identify the various taste and odor in drinking water. Flavor Profile Analysis (FPA), introduced by Metropolitan Water District (MWD) of Southern California in 1980's, used in the food and beverage industry was modified and adapted for use in the drinking water field. FPA determines the specific characteristics of a water sample and the intensity of each individual characteristic, without dilution.

Rules of evidence describing "the scientific method" are used to define presumptive and confirmatory testing procedures to validate the cause of a taste and odor event in drinking water (Mallevialle and Suffet, 1987; Persson, 1992). Figure 2 shows that in determining

the chemical causes of taste and odor problems requires developing a presumptive statistical correlation between the chemical compounds in the water sample and the tastes or odors by sensory panel techniques and separating and identifying those individual compounds that have the same sensory characteristics as the whole water sample, as described by a sensory panel, by sensory GC analysis (Khiari, et al., 1992). Figure 2 shows that final confirmation is completed by having the sensory panels evaluate the chemical identified by FPA.

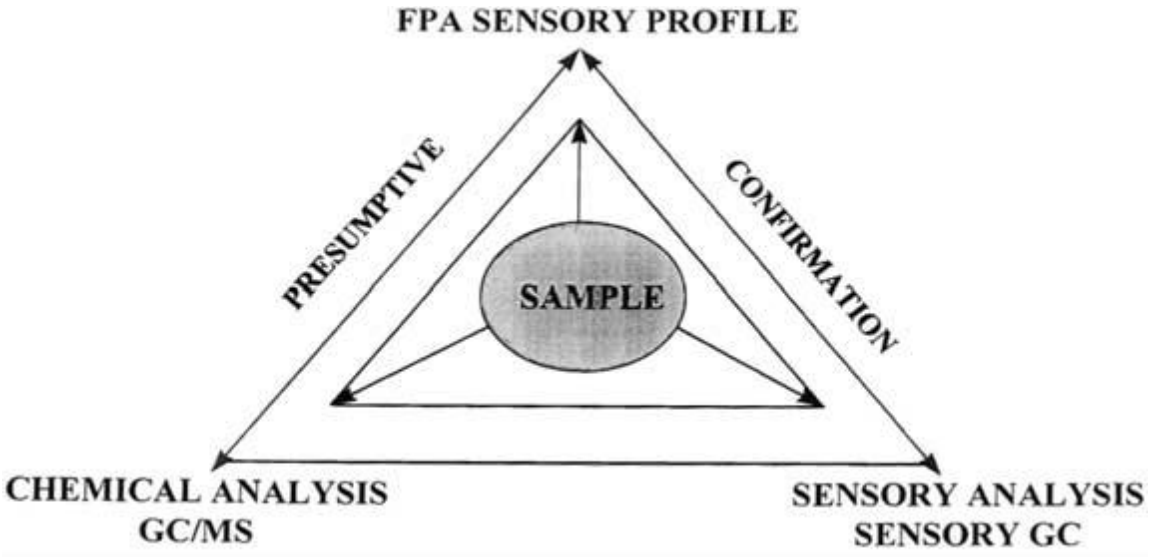


Figure 2 Schematic diagram of relationship between instrument and sensory methods (Khiari, et al., 1992).

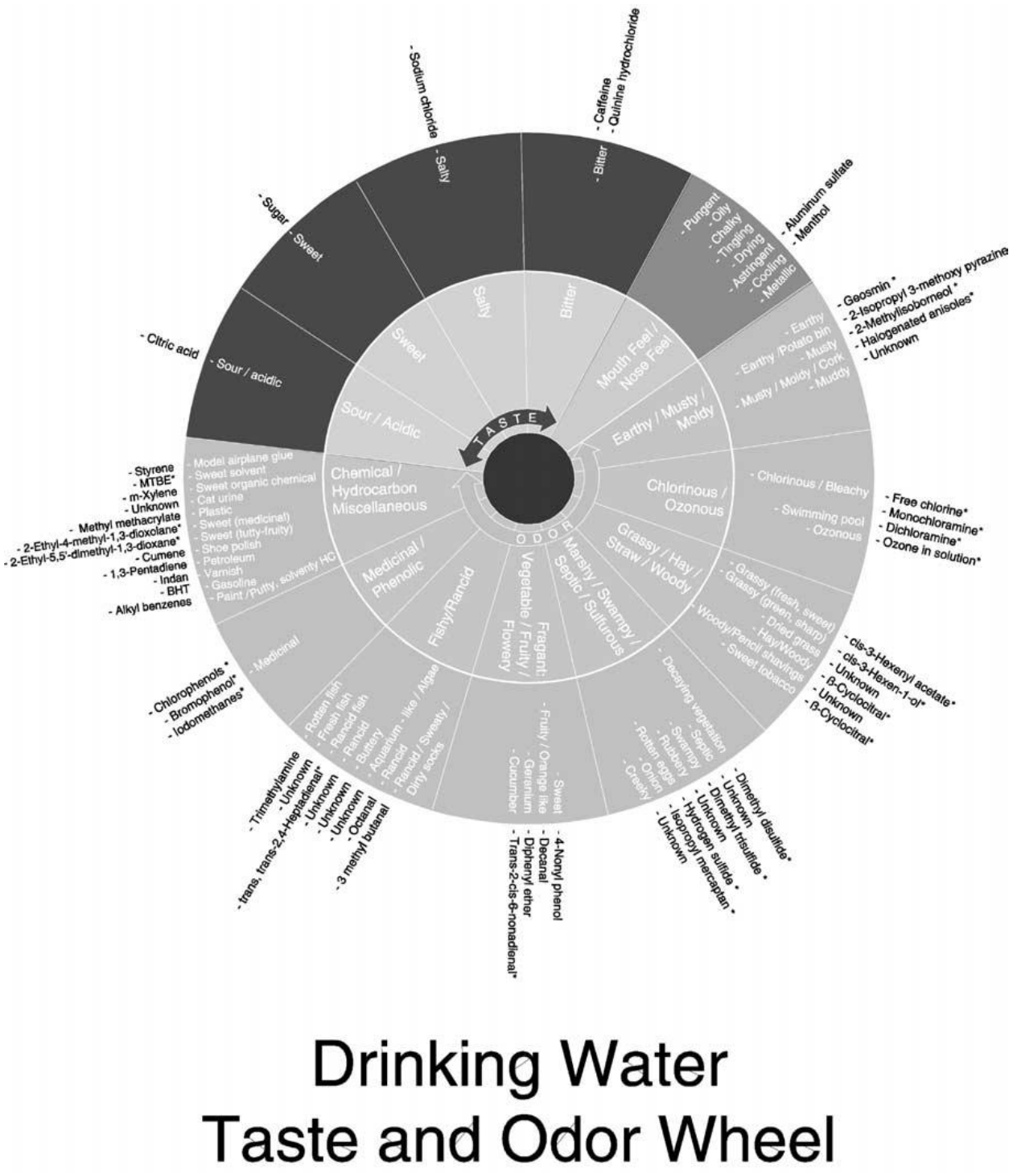
Standard Methods for the Examination of Water and Wastewater (APHA, et al., 2000) includes three methods for evaluating taste and odor The flavor threshold test (FTT), also called threshold odor number (TON), the flavor rating scale (FRS), and flavor profile analysis (FPA). TON consists of performing successive dilutions of the water sample with reference water and comparing each dilution with the reference water. The highest dilution in which odor is perceptible is the TON. A threshold odor number less than or

equal to 3 passes the US and European secondary drinking water standards. The limitations with TON are that no descriptive information about the odor is provided, so this test cannot be used to determine the source or cause of a taste-and-odor event, and upon dilution, the type of odor that is smelled can change and thus the effect of each odor type is not defined.

FPA, unlike TON and FRS, requires no dilution and fewer samples, and is therefore suitable for monitoring source water and the entire treatment process, from raw to finished waters. Since FPA directs panelists to record descriptors for all tastes-and-odors, it the most valuable method for forensic purposes. For each FPA descriptor, a quantitative 7 point scale is used; threshold [0 or 1]; slight [2]; weak [4]; medium [6]; medium strong [8]; strong [10]; very strong [12]. It has been observed that consumers can easily identify an off-flavor in drinking water when a descriptor with an intensity level of above 4, occurs e.g. musty, 4. It is pointed out that individual consumers have different threshold concentration levels and some people are anosmic (i.e., cannot smell) a specific odor. FPA requires only a few panelists to test undiluted samples; however, the panelists have to be highly trained. Once panelists are trained, FPA is a relatively inexpensive method of analysis, and is very quick compared to other methods. The major criticism of FPA besides the requirement for trained panelists is that it is not a statistical method, and is therefore more subjective. Also, certain personality traits (e.g., dominant types) can influence other panelists, and the skill of the FPA leader is essential for leading the panel to consensus. New approaches presently combine statistical methods with FPA. Profile Attribute Analysis (PAA), used in the food and beverage industry, is a statistical method that employs aspects of FPA (Neilson, et al., 1988; Meilgaard, 1999). PAA still requires

consensus, and is based closely on FPA, but with the introduction of numerical scales. Average scores are used instead of arriving at a consensus number and data are analyzed using parametric techniques such as ANOVA. A statistical approach can reduce biases and, in general, give more accurate results. Meilgaard (1999) provides the details for designing and evaluating statistical methods for sensory analysis.

The "Taste and Odor Wheel" developed over the last 20 years includes compounds identified in the eight classes of odorants, four tastes, and one mouth feel/nose feel category. To provide water utilities with the information needed to prevent a taste-and-odor event from occurring, or provide solution to mitigate the problem, it is important to determine the source, including the specified chemical(s) that cause certain tastes and odors. The "Taste and Odor Wheel" helps provide the water utilities with this information. A combination of approaches is still needed to determine the sources of contaminants that cause taste-and-odor problems in drinking water (Suffet, et al., 2004).



Drinking Water Taste and Odor Wheel

Figure 3 Taste and Odor Wheel 2000 (Suffet, et al., 1999)

2.9 **Removal of Off-Flavors**

Organic chemicals such as phenol, hydrogen sulfide and other dissolved gases, soluble substances generated by algae, actinomycetes, and other microorganisms are known to impart objectionable odors to water accompanied by an unpleasant taste. Most materials responsible may be removed by adding activated carbon to the water or passing the water through granular carbon. Other taste and odor control practices consist of mechanical removal of gases through aeration or degasification, and oxidation through chemicals such as chlorine dioxide, hypochlorite, potassium permanganate, and ozone (Kim, et al., 1997).

Geosmin and 2-MIB are relatively stable to chemical and biological degradation and can persist in open water in the dissolved form for some time (Juttener and Watson, 2007). Because of their stability geosmin and 2-MIB are recalcitrant to conventional water treatment, however some conventional physical techniques have been recommended (Krishnani, et al., 2005). Studies have shown that conventional water treatment processes such as coagulation, sedimentation, and filtration are unable to achieve any significant removal of MIB and geosmin (Bruce, et al., 2003; Kutschera, et al., 2009). More advanced treatments, such as granular or powdered activated carbon, ozonation, and membrane filtration can be applied with variable success; their effectiveness is modified by factors such as age of filter beds, type of carbon used, levels of source water dissolved organic material, and proportion of dissolved organic material and proportion of dissolved/particulate geosmin and 2-MIB (Juttener and Watson, 2007). The only treatment methods that have been successfully employed by water treatment plants to remove MIB and geosmin are adsorption by activated carbon or oxidation by strong oxidants such as ozone (Srinivasan and Sorial, 2009). Ferguson, et al., (1990) and Bruce,

et al., (2003) studied and demonstrated MIB and geosmin removal using oxidants such as ozone, hydrogen peroxide, and UV. Addition of chemicals however is expensive and can result in formation of disinfection byproducts, which are unacceptable due to health and regulatory concerns (Cook, et al., 2000).

Juttner (1995) reported that a slow sand filtration unit (flow rate of 420 liters m^{-2} day^{-1}) achieved excellent rates of elimination of geosmin and other terpenoid alcohols. That study found that geosmin was not detectable in the upper layers of the sand filter when this material was removed and chemically extracted, indicating the efficient degradation of this compound by the immobilized microorganisms. This technology has only recently been recognized in North America for its potential application. 2-MIB and geosmin have tertiary alcoholic structures which make the compounds resistant to oxidation. Powdered activated carbon (PAC) can effectively remove MIB and geosmin when the correct dose is applied (Cook, et al., 2000). However, higher doses of PAC were required for both compounds to produce acceptable quality water when turbidities rose above 26 NTU. Ozone and hydrogen peroxide are advanced oxidants that can eliminate 2-MIB, but the efficiency depends on the water quality (Nerenberg, et al., 2000). Using GAC filter and post-ozonation, taste-and-odor compounds were removed below threshold odor number (TON) (Kim, et al., 1997). Another long-term control measure that is used in United States is application of copper sulphate to surface waters to prevent the algal blooms (Sklenar and Horne, 1999). In addition to geosmin and MIB, other compounds such as haloanisoles, pyrazines, beta-cyclocitral and d-limonene can frequently cause unpleasant taste and odor in water supplies.

Although many of the treatment processes mentioned above are quite effective at geosmin and 2-MIB removal, they are often extremely expensive to install, maintain, and operate, particularly where source waters are of poor quality or high in dissolved organics. More long-term proactive management needs to address the source(s) of the problem, by identifying the environmental and biological agents and their controls.

2.10 Other chemicals of environmental concern

Triclosan

Triclosan is included in many consumer products because of its antimicrobial activity. The main use of triclosan is in the formulation of personal care and cosmetic products, therapeutic products and cleaning agents. Other uses of triclosan are in the treatment of textiles and plastics (sportswear, bed clothes, shoes, carpets) to control the growth of disease or odor-causing bacteria (Saurez, et al., 2007). It is also used in the formulation of some oil-based paints. Triclosan was first registered by the EPA in 1969, and currently there are 20 antimicrobial registrations (U.S. EPA, 2008). Triclosan is often detected in the aquatic environment, e.g. waste water, surface water and sediments, and is acutely and chronically toxic to aquatic organisms (Aranami and Readman, 2006).

In developed countries triclosan is typically transported through a waste disposal conveyance system to a sewage treatment facility. Triclosan is well removed in sewage treatment with measured removal rates of 96% for activated sludge plants, 71% for trickling filter plants and 32% for primary treatment plants (McAvoy, et al., 2002). In the United States, approximately 84% of wastewater flow is processed through activated sludge treatment plants, 12% of wastewater flow is processed by trickling filter and 1% by primary treatment (US EPA, 1989).Trace levels of triclosan not removed during wastewater treatment is released to the receiving waters as part of the effluent matrix.

Subsequent loss mechanisms, including degradation in the river, will further reduce environmental concentrations downstream of the effluent discharge point (Morall, et al., 2004).

2, 4 Dichlorophenol

2,4-Dichlorophenol (2,4-DCP) is produced commercially. It is a substituted phenol used in the manufacture of industrial and agricultural products. 2,4-DCP is utilized as the feedstock for the manufacture of the herbicide, 2,4-dichlorophenoxyacetic acid (2,4-D), 2,4-D derivatives (germicides, soil sterilants, etc.) and certain methyl compounds used in mothproofing, antiseptics, and seed disinfectants. 2,4-DCP is also reacted with benzene sulfonyl chloride to produce miticides or further chlorinated to pentachlorophenol, a wood preservative (U.S. EPA, 1980). 2,4-DCP presently has no direct commercial application and is used as an important chemical intermediate, and it is synthesized from dilute aqueous solutions (U.S. EPA, 1980).

2,4- DCP is one of the 129 priority pollutants listed by the U.S. EPA and the major environmental problem is caused by its presence in drinking water and was detected in tap water at various locations in the United States (Tang and Huang, 1996). 2,4-dichlorophenol may occur in the environment from its release from manufacturing industry effluent and its use in chemical industry. Small amounts may also be released from water treatment and wood pulp bleaching chlorination processes and from the degradation of various pesticides in soil. There are believed to be no natural sources of 2,4-dichlorophenol (Avialable at http//www.environment-agency.gov.uk/business/topics/pollution/39415.aspx). A number of physical, chemical, and biological methods have been used to eliminate 2,4-DCP from industrial effluents (Ziagova, 2007).

Acetaminophen

Acetaminophen is the most widely used over-the-counter analgesic in the U. S. with production of 3.6×10^9 g in 2002 (Bedner and Maccrehan, 2006). It is a safe drug when consumed at therapeutic dosages, where the body metabolizes acetaminophen to labile sulfate and glucuronide conjugates for excretion. Consumers spend billions of dollars on prescription drugs and personal care products in the United States (Pontius, 2008). Only 1.4% of Americans return unwanted medicines to pharmacies and more than 35% flush unused drugs down the toilet from which they enter the environment (Burton, 2006). Pharmaceutical compounds such as acetaminophen are detected in the environment are in the range of micrograms per liter to nanograms per liter (Bedner and Maccrehan, 2006; Andreozzi, et al., 2003). Such pharmaceutical products detected in the environment are subjected to wastewater and water treatment plants (Bedner and Maccrehan, 2006). It was reported that atleast 46 million people in the United States are exposed to trace amount of pharmaceuticals in drinking water (Available at, http//www.foxnews.com/story/0,2933,421444,00.html). The United States Geological Survey has already been identified acetaminophen as one of the most frequently detected anthropogenic compounds in a survey of 139 streams in the U.S. (Lu, et al., 2009). Kim, et al., (2007) evaluated the acute aquatic toxicity of several widely used pharmaceuticals including acetaminophen and suggested these compounds pose potential ecological risk. However the effects of these compounds on human health and the environment have not been fully characterized (Onesios, et al., 2008).

Most WWTPs are currently struggling to meet other, very basic challenges in design and capacity (particularly combined stormwater/sewer systems) and are likely to balk at expensive measures without tangible human health benefits (Kehoe, et al., 2007). Studies

have shown that conventional water treatment procedures are only moderately effective in the removal of trace pharmaceuticals (Synder, et al., 2003; Bedner and Maccrehan, 2006). Researchers have examined PPCP removal by biodegradation in many different systems, including WWTPs, membrane bioreactors (MBRs), sequencing batch reactors (SBRs), sand columns, and constructed wetlands. Some of these studies focus solely on biodegradation as a removal process, whereas others examine overall removal due to a combination of processes, including biodegradation (Onesios, et al., 2008). Bedner and Maccrehan, (2006) studied the transformation of acteminophen by chlorination as it is the most widely used chemical process for disinfecting wastewater and drinking water in the U. S.

Atrazine

Atrazine is one of the most used herbicides worldwide (Battaglia, 1989) and about 36,000 metric ton/year are applied only in the U.S.A. (Hileman, 1996). Atrazine is a widely used for control of broadleaf and grassy weeds in corn, sorghum, rangeland, sugarcane, macadamia orchards, pineapple, turf grass sod, asparagus, forestry, grasslands, grass crops, and roses and was used until 1993 for control of vegetation in fallow and in noncrop land (U.S. EPA, 2003). Atrazine was estimated to be the most heavily used herbicide in the United States in 1987/89, with its most extensive use for corn and soybeans in Illinois, Indiana, Iowa, Kansas, Missouri, Nebraska, Ohio, Texas, and Wisconsin (U.S. EPA, 2003). Over 64 million acres of cropland were treated with atrazine in the U.S. in 1990 (Available at http//extoxnet.orst.edu/pips/atrazine.htm).

Atrazine may be released to the environment through effluents from manufacturing facilities and through its use as a herbicide. Residues of atrazine and its metabolites are

commonly found in soils, surface water supplies and groundwater (Crawford, et al., 2000). Atrazine was the second most frequently detected pesticide in EPA's National Survey of Pesticides in Drinking Water Wells (U.S. EPA, 2003). EPA's Pesticides in Ground Water Database indicates numerous detections of atrazine at concentrations above the maximum contamination level (MCL) in ground water in several States, including Delaware, Illinois, Indiana, Iowa, Kansas, Michigan, Minnesota, Missouri, Nebraska and New York. For atrazine the MCL in the U.S.A. is 3 µg/L. An herbicide concentration in frequently high level in the reservoirs is a great concern for public health and aquatic ecosystems (Chung and Gu, 2009). Chronic and harmful effects of atrazine on human health have been previously reported. Atrazine-contaminated drinking water may contribute to higher risks of breast cancer in women (Patlak, 1996; Eldridge, et al., 1994). Conventional water treatment processes are not able to remove atrazine easily (Hallberg, 1996). The use of granular activated carbon (GAC) or powdered activated carbon (PAC) is the treatment method designated by USEPA as the best available technology (BAT) for removing atrazine from drinking water.

2.11 Degradation/Removal of contaminants in environment

Persistence or degradability of compounds in the environment is an important property for proper risk assessment (Rorije and Peijnenburg, 1996). Chemical compounds can be transformed or degraded by a number of different processes and they can be roughly divided into three separate categories namely biodegradation, photochemical transformation initiated by sunlight and chemical transformation (Rorije and Peijnenburg, 1996). Biodegradation is one of the most important processes determining the fate of organic chemicals in the environment (Parsons and Govers, 1990). Photochemical

processes are important transformation pathways for compounds in the gas phase and their contribution to the degradation of compounds present in the soil is generally negligible (Rorije and Peijnenburg, 1996). As far as chemical transformation processes are concerned, they can be roughly subdivided into hydrolysis reaction, oxidation reactions and reduction reactions (Rorije and Peijnenburg, 1996). It is therefore desirable to predict the rate constants of degradation processes especially biodegradation rate constant, oxidation and hydrolysis rate constant, which will prove helpful for determining the risk associated with the compounds.

Biodegradation is the principal abatement process in the environment (Raymond, et al., 2001). It is the most dominant degradative route for various organic chemicals (Peijnenburg, 1994). Biodegradation processes may be distinguished as

- Primary biodegradation; any biologically induced structural transformation in the parent compound alters the molecular integrity.
- Ultimate biodegradation; biological conversion of organic compound to inorganic compounds occur and the products are associated with normal metabolic processes.
- Acceptable biodegradation; biological degradation of an organic compound to the extent that toxicity or other undesirable characteristics are ameliorated.

Factors influencing biodegradation are temperature, population of microorganisms, degree of acclimation, accessibility of metabolic cofactors, cellular transport properties, growth medium, chemical partitioning tendencies and so on (Raymond, et al., 2001).

Oxidation in surface waters is not dominated by a single oxidation process; several oxidants are present at various steady state concentrations (Rorije and Peijnenburg, 1996). Environmental oxidants present in surface water are singlet oxygen, the hydroxyl

radical, and oxyradicals, which can be formed under the influence of sunlight and various other oxidants, can be present depending on the specific environmental conditions (Rorije and Peijnenburg, 1996). The application of ozone in drinking water treatment is widespread throughout the world. Ozone is used for tatste and odor control, decolorization, elimination of micropollutants, disinfection etc. (Gunten, et al., 2003). Ozone decomposes into OH radicals which are the strongest oxidants in water (Gunten, et al., 2003). Disinfection may occur primarily through ozone while oxidation reactions occur through both ozone and OH radicals. Different processes make it difficult to predict the degradation of chemicals in environment. Also, the number of natural or man-made organic compounds present in the biosphere is somewhere between 8 and 16 million molecular species, of which as many as 40 000 are predominant in our daily lives (Hou, et al., 2003). In order to be able to make predictions regarding the fate of chemicals in different environmental compartments, one would have to have various models available, enabling both the calculation of the rate constants of each of the distinct processes mentioned above and the prediction of the products formed. To determine the risk associated with the thousands of chemicals, efforts are made to predict the degradation of chemicals in environment through establishing a reliable structure-activity relationship. Use is made of models that merely require the input of the molecular structure (or properties derived from molecular structure) or physico-chemical properties as the important parameter. Increasing numbers of Quantitative Structure Activity Relationship models are being developed to predict the environmental fate of organic chemicals.

2.12 Quantitative Structure-Activity Relationships in environmental fate processes

Thousands of chemicals must be reviewed by the Environmental Protection Agency to determine toxicological effects to the environment and to human health (Raymond, et al., 2001). The premanufature notices submitted to the EPA for approval often do not contain information regarding degradability of compound (Raymond, et al., 2001). This suggests the need for a method that helps in estimation of degradability of chemicals in environment with little or no dependence on measured input. Among these methods the study of Quantitative Structure Activity Relationships (QSARs) has attracted increasing attention (Peijnenburg, 1994).

The role of QSARs in environmental studies is

- To provide methods for estimation of hazards of contaminants without much dependence on measured input.
- Provide guidelines for chemical classification and to identify outliers.
- Help in understanding the reaction mechanisms (Peijnenburg, 1994).

QSARs have become well established tools in environmental toxicology and chemistry (Parsons and Govers, 1990). However no fundamental theory exists for formulation of QSAR-compatible classes (Peijnenburg, 1994). QSAR from correlation analysis offer a potential approach in predicting reaction rates (Gallagher, 2001). The derivation and application of QSARs require descriptors for molecules (Peijnenburg, 1994). These descriptors are properties or characteristics, inherent to a molecule or to its constituting parts, which together represent the entire molecule (Peijnenburg, 1994). The molecular descriptors may be physico-chemical, geometric, electronic, energy and topological parameters. Electronic structure descriptors represent the number of electrons and

describe the way these are distributed in the molecule and its atom. Some well know electronic structure descriptors are valence connectivity index, electronic charges on atoms, electric moments and polarizability (Peijnenburg, 1994). The exact positions of atoms relative to each other are used to calculate geometric descriptors. Lengthwidth ratio, distance index, van der Waals Volume and steric overlap volume are some of the examples of geometric descriptors. Topological descriptors describe those structural properties of molecules, which do not change when a molecule is deformed without cleavage or superposition of bonds (Peijnenburg, 1994). The number of atoms or of atoms groups and connectivity indices are included in topological descriptors. Electronic energy descriptors specify the electronic energy of atoms, bonds and molecules including the attraction and repulsion of electrons by atoms and molecules (Peijnenburg, 1994). They are calculated by quantum-mechanical methods such as extended Huckel theory, or semi-empirical methods (like MNDO, AM1, CNDO/2). The electronic energy properties include ionization potentials, dipole moments, charge densities, energy of highest occupied molecular orbital (E_{HOMO}), energy of lowest unoccupied molecular orbital (E_{LUMO}).

2.13 Physico-chemical Properties of chemicals

Different chemicals in the environment behave differently and these differences are attributed to physical-chemical properties. The key physicochemical properties are believed to be solubility in water, vapor pressure, octanol-water partition coefficients and dissociation constant in water (Mackay, et al., 1997). Knowing compounds physicochemical properties helps in predicting bioactivity, bioavailability, behavior in

chemical separation, and distribution between environmental compartments (Reinhard and Drefahl, 1998).

Important Physico-chemical Properties

1. Log Octanol-Water Partitioning Coefficient (log K_{ow})

The role of the log-octanol/water partition coefficient (K_{OW}) for organic compounds has been important in predictive environmental studies in the last two decades (Finizio, et al., 1997). Partition coefficient is an indicator of the environmental fate of a chemical since it gives a general idea of how a chemical will be distributed in the environment. Evaluative models use this physico-chemical parameter for the prediction of distribution among environmental compartments to estimate plants and animals bioaccumulation factors (Briggs, et al., 1982). This parameter is also used in predicting the toxic effects of a substance in QSAR studies. Nevertheless the availability of reliable K_{OW} values is still a problem for several compounds (Finizio, et al., 1997).

Definition

The octanol-water partition coefficient, K_{OW}, is defined as

$$K_{OW} = \frac{Concentration \quad in\ octanol\ \ phase}{Concentration \quad in\ aqueous\ \ phase} = \frac{C_O}{C_W} \qquad \text{Equation (2)}$$

where C_O and C_W refer to molar or mass, concentrations in the water-saturated octanol and in the octanol-saturated water phase respectively. The octanol-water partition coefficient (K_{OW}) is a measure of the equilibrium concentration of a compound between octanol and water that indicates the potential for partitioning into soil organic matter (i.e., a high K_{OW} indicates a compound which will preferentially partition into soil organic matter rather than water). K_{OW} is inversely related to the solubility of a compound in water.

Values of K_{OW} are unitless. The parameter is measured using low solute concentrations, where K_{OW} is a very weak function of solute concentration. Values of K_{OW} are usually measured at room temperature (20 ^{0}C or 25 ^{0}C). The effect of temperature on K_{OW} is not great - usually on the order of 0.001 to 0.01 log K_{OW} units per degree, and may be either positive or negative. Measured values of K_{OW} for organic chemicals have been found as low as 10^{-3} and as high as 10^7, thus encompassing a range of ten orders of magnitude. In terms of log K_{OW}, this range is from -3 to 7. The octanol/water partition coefficient is not the same as the ratio of a chemical's solubility in octanol to its solubility in water, because the organic and aqueous phases of the binary octanol/water system are not pure octanol and pure water. At equilibrium, the organic phase contains 2.3 mol/L of water, and the aqueous phase contains 4.5×10^{-8} mol/L of octanol. Moreover, K_{OW} is often found to be a function of solute concentration. The chemical in question is added to a mixture of octanol and water whose volume ratio is adjusted according to the expected value of K_{OW}. Very pure octanol and water must be used, and the concentration of the solute in the system should be less than 0.01 mol/L. The system is shaken gently until equilibrium is achieved (15 min to 1 hr). Centrifugation is generally required to separate the two phases, especially if an emulsion has formed. An appropriate analytical technique is then used to determine the solute concentration in each phase. A rapid laboratory estimate of K_{OW} may be obtained by measuring the retention time in a high-pressure liquid chromatography system; the logarithm of the retention time and the logarithm of K_{OW} have been found to be linearly related. Values of K_{OW} can be considered to have some meaning in themselves, since they represent the tendency of the chemical to partition itself between an organic phase (e.g., a fish, a soil) and an aqueous phase.

Chemicals with low K_{OW} values (e.g., less than 10) may be considered relatively hydrophilic, i.e. they tend to have high water solubilities, small soil/sediment adsorption coefficients, and small bioconcentration factors for aquatic life. Conversely, chemicals with high K_{OW} values (e.g., greater than 10^4) are very hydrophobic (Available at http//pirika.com/chem/TCPEE/LOGKOW/ourlogKow.htm on December, 19, 2009).

In general, a large value means that a chemical tends to be in an organic (non-polar) environment and not in water (polar). The hydrophobicity scale (log K_{OW}) ranges from -2.6 for hydrophilic compounds to +8.5 for hydrophobic compounds (Reinhard and Drefahl, 1998). Most pesticides are less polar than water so they tend to accumulate in soil or living organisms which contain organic matter. So one can see that K_{OW} values give an overall estimate as to where a chemical will be distributed in the environment.

2. Water Solubility

Water solubility (S_W), is the maximum amount of a substance that can dissolve in water at equilibrium at a given temperature and pressure. Water solubility is also known as aqueous solubility. Solubility is measures of the amount of chemical that can dissolve in water. The units of solubility are generally in ppm (parts per -million) which is mg/L (milligrams per liter). It can also be stated in ppb (parts per - billion) which is µg/L (micrograms per liter).

In many environmental studies, this parameter is used to help determine the fate of chemicals in the environment. If a chemical's water solubility is known the distribution of that chemical in the environment and possible degradation pathways can be determined. For example, chemicals that have high solubilities will remain in water and tend to not be adsorbed on soil and living organisms. Water solubility has been correlated

to the octanol/water partition coefficient (K_{OW}), another chemical parameter used to determine the fate of chemicals in the environment. Two of the most important physico-chemical properties relating to the environmental behavior of hydrophobic organic compounds are aqueous solubility and octanol-water partition coefficient (Pontolillo and Eganhouse, 2001).

Aqueous/Water solubility (S_W) is defined as the equilibrium distribution of a solute between water and solute phases at a given temperature and pressure. Because S_W is the maximum solute concentration possible at equilibrium, it can function as a limiting factor in concentration dependent (for example, kinetic) processes (Pontolillo and Eganhouse, 2001).

3. Henry's Law Constant

A commonly used method for quantifying the solubility of a gas in a liquid is Henry's law, which asserts that the solubility of a solute (gas) in a solvent (liquid) is proportional to the solute's gas phase partial pressure (Cichowski, et al., 2005). Henry's Law determines the extent, which the odorant molecules can dissolve. Henry's Law states that the solubility of a gas in liquid is a function of the partial pressure of the gas above that liquid. In other terms, the concentration of the gas in the liquid is proportional to the concentration in the atmosphere with the Henry's Law Constant (HLC) describing the relationship.

Chemicals with a high HLC tend to volatilize from water and be distributed in the atmosphere. A chemical with a low HLC will tend to accumulate in water and soil, rather than volatilize. This can be an environmental concern since the accumulation of chemicals in water can have adverse effects upon living organisms. Chemicals in the air

can partition (move) into water droplets in clouds and fog. If the HLC is low, substantial amounts of the volatilized chemical will dissolve in the water droplets and be transported back to the earth's surface by rain. This process of a chemical moving from the gas phase into water droplets and being deposited onto the earth's surface is called wet deposition. Dry deposition is another process that occurs when the chemical is adsorbed onto soil particles in air which is deposited on the earth's surface.

4. Log Octanol-Air Partition Coefficient (K_{OA}) (EPI SUITE User's Guide)

The octanol-air partition coefficient (K_{OA}) is the ratio of a chemical's concentration in octanol to the concentration in air at equilibrium. It is useful for predicting the partitioning behavior between air and environmental matrices such as soil, vegetation, and aerosol particles. Various models utilize K_{OA} to screen and rank chemicals for environmental persistence and long-range transport. At present, experimentally determined K_{OA} values are available for only several hundred compounds. Therefore, the ability to estimate K_{OA} is necessary for screening level evaluation of most chemicals.

5. Soil Adsorption Coefficient (K_{OC})

Adsorption of chemicals on soils or sediments is a major factor in the transportation and eventual degradation of chemicals. Water solubilizes polar chemicals because it can bond with them more easily. Chemicals that are non-polar tend to be pushed out of water and onto soils which contain non-polar carbon material. Soils vary in the amount of organic carbon content, which is mainly what determines the amount of pesticide adsorbed. K_d is called the sorption coefficient and it measures the amount of chemical adsorbed onto soil per amount of water. Values for K_d vary greatly because the organic content of soil is not

considered in the equation. The preferred value for determining a soil's ability to adsorb is soil adsorption coefficient (K_{OC}), since it considers the organic content of the soil. The soil adsorption coefficient, K_{OC}, is crucial for estimating a chemical compound's mobility in soil and the prevalence of leaching from soil. The adsorption of a compound increases with an increase in organic content, clay content, and surface area of the soil. The presence of a chemical compound can also be detected in ground water, and inference can be made about its residence time in the soil and the degradation period before reaching the water table. The presence of continuous pores or channels in soil will increase the mobility of a chemical compound in the soil.

K_{OC} can be defined as "the ratio of the amount of chemical adsorbed per unit weight of organic carbon (OC) in the soil or sediment to the concentration of the chemical in solution at equilibrium" (Lyman, 1990). It is represented by the following equation (Lyman, 1990)

$$K_{OC} = \frac{\mu g\ adsorbed\ /_{g\ organic\ \ carbon}}{\mu g\ /_{ml\ solution}} \qquad \text{Equation (3)}$$

The units of K_{OC} are typically expressed as either L/kg or mL/g.

K_{OC} provides an indication of the extent to which a chemical partitions between solid and solution phases in soil, or between water and sediment in aquatic ecosystems. Estimated values of K_{OC} are often used in environmental fate assessment because measurement of K_{OC} is expensive. Traditional estimation methods rely upon the octanol/water partition coefficient or related parameters, but the first-order molecular connectivity index (MCI)

has been used successfully to predict K_{OC} values for hydrophobic organic compounds (Sabljic, 1984, 1987; Bahnick and Doucette, 1988).

6. Vapor Pressure

Vapor Pressure is defined as the pressure that a chemical in the gas phase exerts over a surface. This surface can be water or dry soil. At room temperature, vapor pressure values can range from 10^{-5} to 300 mm of Hg (mercury).Vapor pressure units are generally expressed in three ways mm Hg (millimeters of mercury), Pa (pascals), atm (atmospheres). The unit mm of Hg is a measure of the pressure exerted by a gas on a mercury surface which pushes the mercury level up so many mm (millimeters). The atmospheric pressure on an average day is 760 mm Hg. One atm is defined as the pressure exerted by a column of mercury 760 mm high at 0°C. If the pressure is 0.95 atm, then it is said that the pressure is 95% of that exerted by a mercury column 760 mm Hg high. Pascals (Pa) is the preferred unit for pressure and is generally in the form MPa (Mega-Pascals). The relationship between the three units is

1 atm = 760 mm Hg = 101325 Pa = 0.1 MP

1 MPa = 106 Pa

7. Enthalpy of vaporization

The enthalpy of vaporization of liquids and subcooled liquids at 298 K (ΔH_{VAP}) is an important parameter in environmental fate assessments that consider spatial and temporal variability in environmental conditions (Macleod, et al., 2007).The enthalpy of vaporization is the heat of vaporization for vaporizing one mole of the substance under three specific conditions (1) the pressure remains constant, (2) the only possible work that

occurs is expansion against the atmosphere and (3) the temperature remains constant during the process.

The enthalpy of vaporization ΔH_{VAP} is defined as the difference between the vapor and liquid-phase enthalpies at a given temperature and the corresponding saturated vapor pressure.

8. Frontier Orbital Energies E_{HOMO} and E_{LUMO}

The chemical reaction between two molecular species is always accompanied by a rearrangement of electron density. For a given pair of two reacting agents, the more electronegative compound will gain some electronic charge upon forming a covalent bond with the reaction partner, which, in turn, loses the respective amount of electron density. The general tendency of molecule to gain or lose electronic charge may serve as a global reactivity parameter in the context of QSAR investigation (Cronin and Livingstone, 2004).

The ionization energy or ionization potential is the energy necessary to remove an electron from the neutral atom. The ionization energy can be thought of as a kind of counter property to electronegativity in the sense that low ionization energy implies that an element readily gives electrons to a reaction, while a high electronegativity implies that an element strongly seeks to take electrons in a reaction. The electron affinity is a measure of the energy change when an electron is added to a neutral atom to form a negative ion (Nave, 2006).

To characterize the global readiness of molecules to donate or accept electron charge, the lowest ionization potential and the greatest electro affinity (that are simply the ionization potential and electron affinity) would be the best parameters to model reactions for

nucleophilic and electrophilic interactions of a compound with endogenous reaction partners. The associated molecular orbital energies according to Koopman's theorem, can be regarded as approximations of a compound's ionization potential (IP) and electron affinity (EA) respectively. These are frontier orbital energies of the highest occupied molecular orbital (E_{HOMO}) and lowest unoccupied molecular orbital (E_{LUMO}), shown in equations 2 and 3 (Cronin and Livingstone, 2004).

$IP = - E_{HOMO}$ Equation (4)

$EA = - E_{LUMO}$ Equation (5)

2.14 Relationship between molecular descriptors and degradation rate constants (Biodegradation, oxidation and hydrolysis rate constants)

Application of Quantitative Structure Activity relationship in environmental toxicology and chemistry has been well established and there have been increasing interest in the study of biodegradation and molecular structure relationship (Parsons and Govers, 1988). The most usual approach is the correlation of biodegradation rate data with molecular descriptors such as physic-chemical properties, electronic parameters or structural parameters. Descriptors such as partition coefficients that describe the hydrophobicity and reverse phase HPLC retention time are most commonly used in QSARs for biodegradation (Parsons and Govers, 1988). A study by Banerjee et. al (1984) showed the decrease in biodegradation rate constants with increase in n-octanol-water partition coefficient for chlorinated phenols, anisoles and resorcinols. Paris, et al., (1982) studied the correlation of biodegradation rate constant and various physic-chemical properties such and pK_a, the Hammett substituent parameter, the Taft's steric parameter, log K_{OW}, and the van der Waals radii. In this study the best results were obtained with van der Waals radii suggesting the biodegradation rate of the compounds studied are controlled

by steric properties of the substituents which may affect the binding of these compounds to enzymes. Many of the published correlations associating structure and molecular activity to biodegradation typically quantify the degradability of a limited set of homologous chemicals, while for compounds displaying varying chemical structures these correlations are scarce. (Raymond, et al., 2001). Correlations for homologous compounds are represented by a simple linear or quadratic equations that includes one or molecular descriptors which are selected based on their ability to fit the measured data (Raymond, et al., 2001). First-order biodegradation rate of 12 pesticides of various structures were correlated parabolically with their octanol-water partition coefficient (R^2 = 0.697) and linearly with their alkaline hydrolysis rate constant (R^2= 0.454) by Kanazawa (1987).

Chemical oxidation using ozone has been proved to be an effective treatment process for a wide spectrum of organic micropollutants during bench, pilot and full-scale experiments in both wastewater and drinking water (Broséus, et al., 2009). Due to its high oxidation potential, ozone treatment is widely used in drinking water treatment for disinfection, color removal, taste and odor control, decrease of disinfection by-products formation, biodegradability increase and also for the successful degradation of many organic contaminants (Broséus, et al., 2009). Ozone reacts with organic contaminants through both a direct reaction with molecular ozone or through indirect reactions with free radicals (including the hydroxyl radical OH) produced by the decomposition of ozone and the rate of OH radical formation depends on the water matrix, especially its pH, alkalinity, type and content of natural organic matter (Gunten, 2003). Molecular ozone reacts selectively with unsaturated bonds, aromatic systems and amino groups

whereas the reaction with OH radicals is a faster and unselective process (Broséus, et al., 2009). To assess the removal efficiency of ozonation, it is necessary to determine the rate constants for the reaction of micropollutants with ozone and OH radicals. The rate constant indicates the reactivity of a reaction, and it becomes of vital importance when deciding whether ozonation is an economically sound option for removing contaminants from raw water during drinking water treatment (Hu, et al., 1999). Estimation of rate constants during oxidation processes are made from the chemical properties in recently developed QSARs (Hu, et al., 1999).

Molecular descriptors such as oxidation potentials, σ constants in the Hammett equation, and molecular orbital energies are employed to correlate with oxdation rate constants of the compounds (Hu, et al., 1999). The σ constant in the Hammett equation is the one most commonly used for QSAR analysis of reactivity of compounds in the oxidation process. For example, the kinetics of the heterogeneous ozonation of o,p-activated aromatic organic compounds (Gould, 1987) and substituted phenols (Hoigne and Bader, 1983) have been successfully correlated with their σ constants. Half-wave potentials have also been employed for QSAR analysis of oxidation rate constants of the reaction between substituted phenols with single oxygen, chlorine dioxide, and manganese (III/IV) oxides (Rorije and Peijnenburg, 1996). However, the use of half-wave potentials as descriptors has a disadvantage because of the limited availability of consistent sets of this descriptor (Rorije and Peijnenburg, 1996). Recently, the energy of the highest occupied molecular orbital (E_{HOMO}) has been used to estimate the kinetic parameters of oxidation of organic compounds (Hu, et al., 1999). Studies on E_{HOMO} based correlation include oxidation of phenols and anilines by H_2O_2 catalyzed by horseradish peroxidase

compound II (Sakurada, et al., 1990) and oxidation of hydrofluorocarbons and hydrofluoroethers by hydroxyl radicals (Cooper and Cunningham, 1992; Percival et al., 1995; Bartolotti and Edney, 1994). Gallagher, et al., (2001) used various descriptors such as diffusion coefficients, solubilities, sediment-water partion coefficients, and vapor pressure for predicting the dechlorination rate of chlorinated alkanes and alkenes. However these descriptors yielded correlation coefficients (R^2) of less than 0.5. Later in this study theoretically derived structure-based descriptors, including quantum-chemistry calculations using the semiempirical method (MOPAC) was used. The energy of the lowest unoccupied molecular orbital (E_{LUMO}) provided the best correlations to the log of the dechlorination rate constant with an R^2 value of 0.85. The fact that E_{HOMO} and E_{LUMO} can be readily calculated for almost all environmentally important compounds by using a standard technique of computational chemistry is a great advantage of E_{HOMO} and E_{LUMO} over other predictors.(Hu, et al., 1999).

CHAPTER III

METHODOLOGY

3.1 Data Sources for Physicochemical Properties of chemicals

Different chemicals in the environment behave differently and these differences are attributed to physical-chemical properties. The key physicochemical properties are believed to be solubility in water, vapor pressure, octanol-water partition coefficients and dissociation constant in water (Mackay, et al., 1997). Knowing compounds physicochemical properties helps in predicting bioactivity, bioavailability, behavior in chemical separation, and distribution between environmental compartments (Reinhard and Drefahl, 1998). The biodegradation rates, oxidation rates and hydrolysis rates are believed to be the important property for persistence or degradability of compounds in environment (Rorije and Peijnenburg, 1996). It is therefore desirable to predict these rate constants to assess the fate of compounds in environment. These degradation rate were related to physical-chemical properties of compounds, for the advantage of this approach is, once an acceptable model is developed, is the ability to predict relative or absolute degradation rates strictly on the basis of the compound structure without laboratory testing other than the calibration data set.

Determining various physicochemical properties for each compound experimentally would prove to be costly and time consuming. Physical-chemical properties of geosmin, 2-methylisoborneol, acetaminophen, triclosan, 2,4-dichlorophenol and atrazine have been previously studied and calculated in relevant literature. For these compounds physical-chemical properties available in literature were used as part of data. Properties like log octanol/air partition coefficient, soil partition coefficient were calculated using Estimation Program Interface Suite (EPI Suite v. 4.00) developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC). Quantum chemical properties such as energy of highest occupied molecular orbital (E_{HOMO}) and energy of lowest unoccupied molecular orbital (E_{LUMO}) were calculated using Molecular Modeling Pro software's, Molecular Orbital Package (MOPAC), a sub routine software of Molecular modeling Pro, in which, the AM1 SCF (Self consistent field) semiempirical method implemented in the software was used. AM1 (Austin Model 1) is an popular semiempirical method that uses the parameterized functions that allow a substantially simplified and in particular much faster calculations of the properties and total electronic energy can be obtained using the self consistent field (SCF) (Cronin and Livingstone, 2004).

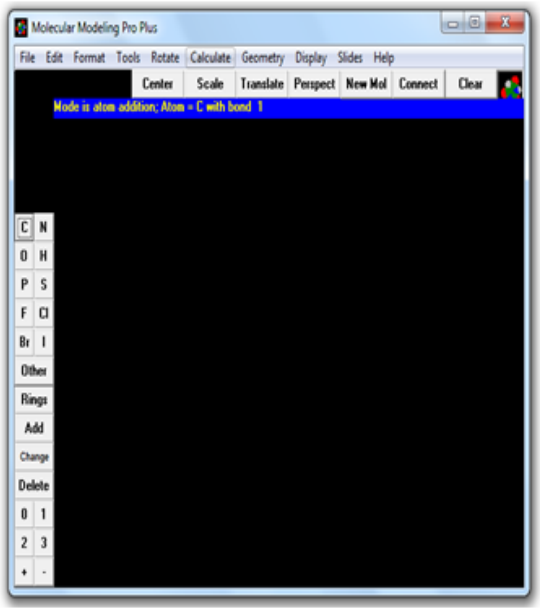
Estimation Program Interface Suite (EPI)

Estimation Program Interface Suite was available from the EPA website. The software was run on computer with Windows operating system. A single simplified molecular input line entry specification (SMILES) of the chemical whose physical-chemical property needs to be calculated was the only input parameter. The SMILES notations were available from www.daylight.com. The values of log octanol-air partition

coefficient and log soil adsorption coefficient calculated from EPI Suite was used in the study.

Molecular Modeling Pro:

The Molecular Modeling Pro program uses the computational chemistry method for calculation of various physical properties of chemicals. Molecular Modeling Pro software was available from Chem SW. The software was installed and run on computer with Windows operating system. The input parameter to calculate the energy of molecular orbital, molecular file (MDL.mol file) was used. A MDL Molfile is a file format holding information about the atoms, bonds, connectivity and coordinates of a molecule. The molfile consists of some header information, the Connection Table (CT) containing atom info, then bond connections and types, followed by sections for more complex information. The molfile is sufficiently common that most, if not all, cheminformatics software systems/applications are able to read the format. The chemical structures for all the six compounds as MDL.mol file were available to download from www.chemicalbook.com. The molfiles were opened in Molecular Modeling Pro program using the file menu option Open new molecule. Figure 4 explains the process of inputting the chemical in Molecular Modeling Pro.



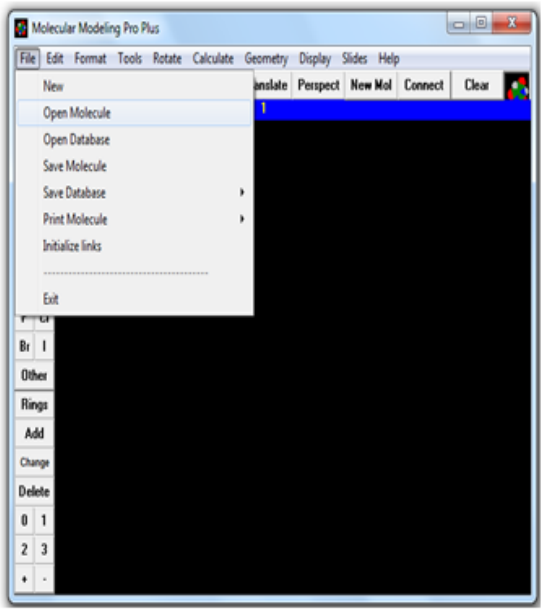
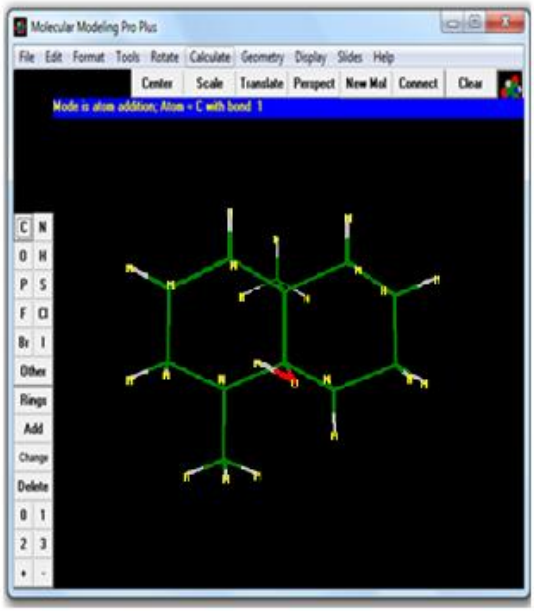


Figure 4 (a) Figure 4(b)

Figure 4 (a) Molecular Modeling Pro program screen.

Figure 4 (b) Step to open a molecule in Molecular Modeling Pro

After the chemical was imported as a .mol file, Molecular Orbital Package (MOPAC) was run with keywords AM1, SCF, and VECTORS to calculate the energies of highest occupied (E_{HOMO}) and lowest unoccupied (E_{LUMO}) molecular orbital's (Stewart, 2000). MOPAC is a subroutine program which is available in the tools menu of the Molecular Modeling Pro program. Figure 5 and 6 explains the steps to run MOPAC. The output is in the form of a word file, an example of which is presented in APPENDIX A, for geosmin.



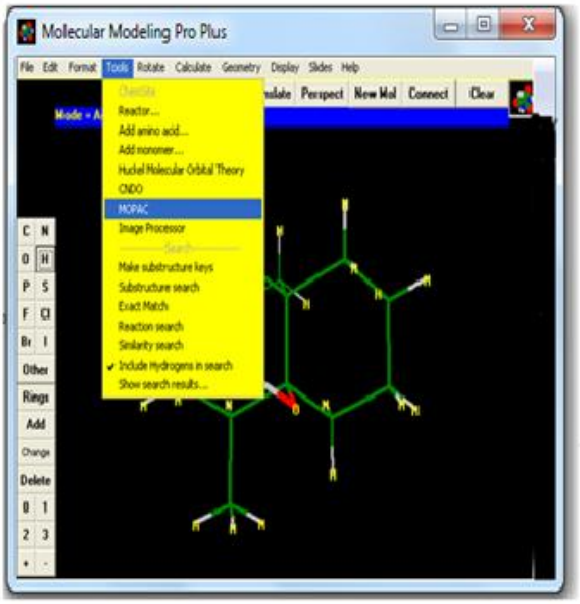


Figure 5 (a) Figure 5 (b)

Figure 5 (a) Geosmin.mol file opened in Molecular Modeling Pro

Figure 5(b) MOPAC executed in Molecular Modeling Pro program

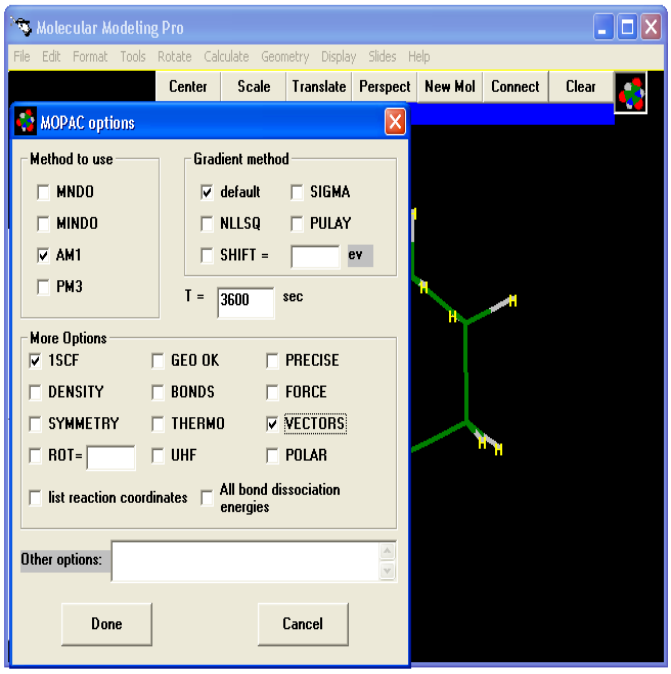


Figure 6 Running MOPAC with keywords

To confirm the accuracy of the molfiles, results from the software (E_{HOMO} and E_{LUMO} values) were validated by making comparisons with the E_{HOMO} and E_{LUMO} values of chemicals that were available in literature (Niu, 2004; Xuejun, 2004, Chen, 1996). The values were all within 20% when compared with the literature value and many were much close. These are presented in Table 6 below.

Table 6 Comparison of E_{HOMO} and E_{LUMO} values.

Chemical Name	E_{HOMO} (Calculated)	E_{HOMO} (Literature)	E_{LUMO} (Calculated)	E_{LUMO} (Literature)
Anthracene	-7.86086	-8.248	-1.08445	-0.970
Para-chloro benzonitrile	-8.25645	-9.0004	0.24563	0.2420
Naphthalene	- 8.50559	-8.918	-0.45225	-0.361
2-biphenyl	-8.76252	-8.835	-0.34406	-0.408

The physical-chemical properties used as descriptors in this study are molecular weight, log octanol/water partition coefficient (Log K_{OW}), solubility in water, vapor pressure, Henry's law constant, log octanol/air partition coefficient (Log K_{oa}), soil adsorption coefficient (K_{OC}), enthalpy of vaporization, energy of highest occupied molecular orbital (E_{HOMO}) and energy of lowest unoccupied molecular orbital (E_{LUMO}). The values of descriptors are summarized in Chapter 4.

3.2 Degradation Rates of Chemicals

The biodegradation rates, oxidation rates and hydrolysis rates of geosmin, 2-methylisoborneol, acetaminophen, triclosan, 2,4-dichlorophenol and atrazine were

extracted from various literature. The following paragraph summarizes the studies from which the three rate constants were extracted

Hoefel, et al., (2009) studied the biodegradation of geosmin caused by Gram-negative bacterium, Geo48, from the biofilm of a water treatment plant sand filters. Ho, et al., (2006), reported biological sand filtration to be an effective process for the complete removal of MIB and geosmin, with removal shown to be predominantly through biodegradation. The bacterial consortium effectively biodegraded 2-chlorophenol, 3-chlorophenol and 2,4-dichlorophenol in a study by Herrera, et al., (2006) The biodegradation kinetics of 2,4-dichlorophenol (2,4-DCP) by culture acclimated to mixture of 4-chloropheno (4-CP) and 2,4-DCP and the culture acclimated to 4-CP only were investigated in aerobic batch reactors by Sahinkaya and Dilek, (2006). In this study isolated pure strains from mixed cultures were searched for their ability towards the biodegradation of 2,4-DCP. In situ microcosms (ISM) and laboratory batch microcosms (LBM) were used for determination of the first-order degradation rate constants of 2,4 – dichlorophenol by Neilsen, et al., (1996). Ziagova, et al., (2007) studied the kinetics of 2,4-dichlorophenol degradation by *Pseudomonas sp.* cultures in the presence of glucose. Lu, et al., (2009) studied the removal of acetaminophen which followed second-order kinetics with first-order to the concentrations of both the substrate and the enzyme. Hansveit and Hamwijk, (2003) studied the biodegradation of triclosan which followed first-order kinetics with CO_2 evolution. Crawford, et al., (2000) studied the the biodegradation of atrazine under different redox conditions in the presence and absence of an electron donor (glucose) and electron acceptors (oxygen, NO_2). The values of the

biodegradation rate constants extracted from the studies mentioned above is summarized in later chapters (Refer table 12).

Peter and Gunten, (2007) studied the applicability of ozonation to mitigate taste and odor problems in drinking water. Second-order rate constants of eleven taste and odor compounds (geosmin and 2-methylisoborneol) with ozone and hydroxyl radicals were determined under laboratory conditions. Tang and Huang, (1996) studied the oxidation kinetics and mechanism of 2,4-dichlorophenol by Fentons reagent; while advanced oxidation processes (AOPs) using UV, UV/H_2O_2, Fenton and photo-Fenton treatment were investigated at laboratory scale for aqueous solutions of 2,4-dichlorophenol (DCP) by Momani, et al., (2003). Benitez, et al., (2000) studied the oxidation of 2,4-DCP by ozone. Oxidation of the antimicrobial agent triclosan by aqueous ozone was investigated by Suarez, et al., (2007). Latch, et al., (2005) and Arnold, et al., (2003) studied the reaction of triclosan with hydroxyl radicals. Oxidation of atrazine with ozone and hydroxyl radicals were studied by Hoigne and Bader, (1983) and Scholles and Willson, (1967). The values of all the three rate constants are summarized in Chapter 4.

The correlation between the descriptors (physical chemical properties found in literature and calculated by the software) and the rate constants (biodegradation, oxidation and hydrolysis) were determined by plotting graphs in Microsoft Excel. The following correlations were made

- Biodegradation rate vs. Molecular Weight
- Biodegradation rate vs. Log K_{OW}
- Biodegradation rate vs. Water Solubility
- Biodegradation rate vs. Henry's Law Constant
- Biodegradation rate vs. Log Octanol Air Partition Coefficient
- Biodegradation rate vs. Soil Adsorption Coefficient
- Biodegradation rate vs. Enthalpy of Vaporization
- Biodegradation rate vs. Vapor Pressure
- Biodegradation rate vs. LUMO
- Biodegradation rate vs. HOMO
- Log Oxidation rate vs. Molecular Weight
- Log Oxidation rate vs. Log K_{OW}
- Log Oxidation rate vs. Water Solubility
- Log Oxidation rate vs. Henry's Law Constant
- Log Oxidation rate vs. Log Octanol Air Partition Coefficient
- Log Oxidation rate vs. Soil Adsorption Coefficient
- Log Oxidation rate vs. Enthalpy of Vaporization
- Log Oxidation rate vs. Vapor Pressure
- Log Oxidation rate vs. LUMO
- Log Oxidation rate vs. HOMO
- Hydrolysis rate vs. Molecular Weight
- Hydrolysis rate vs. Log K_{OW}
- Hydrolysis rate vs. Water Solubility
- Hydrolysis rate vs. Henry's Law Constant
- Hydrolysis rate vs. Log Octanol Air Partition Coefficient
- Hydrolysis rate vs. Soil Adsorption Coefficient
- Hydrolysis rate vs. Enthalpy of Vaporization
- Hydrolysis rate vs. Vapor Pressure
- Hydrolysis rate vs. LUMO
- Hydrolysis rate vs. HOMO

The R-squared value was calculated from the graphs plotted using simple linear regression lines using Microsoft Excel. The results are presented and discussed in Chapter 4 and the conclusions based on the correlations (R2) are discussed in Chapter 5.

CHAPTER IV

RESULTS AND DISCUSSION

4.1 Properties of chemicals used as descriptors

Data extracted from various relevant literature and data which was produced using the Estimation Program Interface (EPI) Suite and MOPAC software are presented in this chapter. The physicochemical properties of geosmin, 2-methylisoborneol, 2,4-dichlorophenol, triclosan, acetaminophen and atrazine are presented in Tables 6 through 11, respectively. The source from which the data was extracted or calculated is also presented in the tables. The values of E_{HOMO} and E_{LUMO} are calculated using MOPAC for all the six compounds. The log octanol-air partition coefficient and log soil adsorption coefficient for all compounds were calculated using EPI Suite. The log soil adsorption coefficient for 2,4-dichlorophenol was available in literature and was used in the study. The enthalpies of vaporization for all compounds were available from Advanced Chemistry Development Labs (ACD/Labs) website, which is commercial service for instant access to chemical databases and property predictions programs.

Table 7 Physicochemical Properties of Geosmin

No	Properties	Geosmin	Reference
1	Log Octanol/water partition coefficient Log K_{OW}	3.57	Nakamura et al, (2001)
2	Solubility in Water (mg/L)	150.20	Pirbazari et al., 1992
3	Boiling Point (^{0}C)	270	Gerber (1967)
4	Melting Point (^{0}C)	47.08	Calculated using EPI Suite
5	Vapor Pressure (atm, 25^{0}C)	5.49×10^{-5}	Pirbazari et al., (1992)
6	Henry's Law Constant (atm-m^3/mole, 25^{0}C)	1.05×10^{-4}	Pirbazari et al., (1992)
7	Log Octanol-Air Partition Coefficient (Log K_{oa})	6.88	Calculated using EPI Suite
8	Soil Adsorption Coefficient (Log K_{OC})	2.48	Calculated using EPI Suite
9	Enthalpy of Vaporization (kJ/mol)	59	Advanced Chemistry Development Lab Inc. Database.
10	Energy of Highest Occupied Molecular Orbital (eV)	-10.46	Calculated using MOPAC
11	Energy of Lowest Unoccupied Molecular Orbital (eV)	2.96	Calculated using MOPAC

Table 8 Physicochemical Properties of 2-Methylsioborneol

No	Properties	2-Methylisoborneol	Reference
1	Log Octanol/water partition coefficient (Log K_{OW})	3.13	Song et al, 2007
2	Solubility in Water (mg/L)	194.50	Song et al, 2007
3	Boiling Point (^{0}C)	196.70	Song et al, 2007
4	Melting Point (^{0}C)	31.00	Calculated using EPI Suite
5	Vapor Pressure (mm of Hg, 25^{0}C)	55.17×10^{-3}	Pinar et al, 2005
6	Henry's Law Constant (atm-m^3/mole, 25^{0}C)	1.149×10^{-4}	Pinar et al, 2005
7	Log Octanol-Air Partition Coefficient (Log K_{oa})	6.75	Calculated using EPI Suite
8	Soil Adsorption Coefficient (Log K_{OC})	2.35	Calculated using EPI Suite
9	Enthalpy of Vaporization (kJ/mol)	51.80	Advanced Chemistry Development Lab Inc. Database.
10	Energy of Highest Occupied Molecular Orbital (eV)	-9.17	Calculated using MOPAC
11	Energy of Lowest Unoccupied Molecular Orbital (eV)	2.32	Calculated using MOPAC

Table 9 Physicochemical Properties of 2,4 Dichlorophenol

No	Properties	2, 4 Dichlorophenol	Reference
1	Log K_{OW}	3.34	Dean et al, 1996
2	Solubility in Water (mg/L)	4500.00	Bhatnagar et al, 2009
3	Boiling Point (^{0}C)	210.00	Bhatnagar et al, 2009
4	Melting Point (^{0}C)	45.00	Bhatnagar et al, 2009
5	Vapor Pressure (mm of Hg, 25^{0}C)	12×10^{-2}	Spectrum Lab Chemical Fact Sheet
6	Henry's Law Constant (atm-m^3/mole, 25^{0}C)	4.29×10^{-6}	Bhatnagar et al, 2009
7	Log Octanol-Air Partition Coefficient (Log K_{oa})	7.70	Calculated using EPI Suite
8	Soil Adsorption Coefficient (Log K_{OC})	2.20	US EPA, 1980.
9	Enthalpy of Vaporization (kJ/mol)	46.50	Advanced Chemistry Development Lab Inc. Database.
10	Energy of Highest Occupied Molecular Orbital (eV)	-6.49	Calculated using MOPAC
11	Energy of Lowest Unoccupied Molecular Orbital (eV)	0.82	Calculated using MOPAC

Table 10 Physicochemical Properties of Triclosan

No	Properties	Triclosan	Reference
1	Log K_{OW}	4.80	Kumar et al, 2009
2	Solubility in Water (mg/L)	10.00	Kumar et al, 2009
3	Boiling Point (^{0}C)	200.00	JEEN INT. CORP, MSDS
4	Melting Point (^{0}C)	54.00 ^{0}C to 57.30 ^{0}C	Merck Index, 1983
5	Vapor Pressure (mm of Hg, 25^{0}C)	4.60×10^{-6}	Merck Index, 1983
6	Henry's Law Constant (atm-m^3/mole, 25^{0}C)	5×10^{-9}	PBT Profiler (2004)
7	Log Octanol-Air Partition Coefficient (Log K_{oa})	6.75	Calculated using EPI Suite
8	Soil Adsorption Coefficient (Log K_{OC})	2.35	Calculated using EPI Suite
9	Enthalpy of Vaporization (kJ/mol)	61.20	Advanced Chemistry Development Lab Inc. Database.
10	Energy of Highest Occupied Molecular Orbital (eV)	-5.62	Calculated using MOPAC
11	Energy of Lowest Unoccupied Molecular Orbital (eV)	0.52	Calculated using MOPAC

Table 11 Physicochemical Properties of Acetaminophen

No	Properties	Acetaminophen	Reference
1	Log K_{OW}	0.48	Carlsson and Karlberg, 2000
2	Solubility in Water (mg/L)	1.40×10^{4}	Yalkowsky et al, 1980
3	Boiling Point (^{0}C)	340.65	Calculated using EPI Suite
4	Melting Point (^{0}C)	170.00	CRC handbook
5	Vapor Pressure (mm of Hg, 25^{0}C)	1.94×10^{-6}	Calculated using EPI Suite
6	Henry's Law Constant (atm-m^3/mole, 25^{0}C)	1.27×10^{-11}	Calculated using EPI Suite
7	Log Octanol-Air Partition Coefficient (Log K_{oa})	11.04	Calculated using EPI Suite
8	Soil Adsorption Coefficient (Log K_{OC})	1.32	Calculated using EPI Suite
9	Enthalpy of Vaporization (kJ/mol)	66.20	Advanced Chemistry Development Lab Inc. Database.
10	Energy of Highest Occupied Molecular Orbital (eV)	-5.53	Calculated using MOPAC
11	Energy of Lowest Unoccupied Molecular Orbital (eV)	-0.49	Calculated using MOPAC

Table 12 Properties of Atrazine

No	Properties	Atrazine	Reference
1	Log K_{OW}	2.60	Hansch et al. 1995
2	Solubility in Water (mg/L)	34.70	Ward and Weber, 1968
3	Boiling Point (^{0}C)	313.03	Calculated using EPI Suite
4	Melting Point (^{0}C)	173 ^{0}C to 175 ^{0}C	HSDB 2002
5	Vapor Pressure (mm of Hg, 25^{0}C)	2.89×10^{-7}	Tomlin 1997
6	Henry's Law Constant (atm-m^3/mole, 25^{0}C)	2.96×10^{-9}	Riederer 1990
7	Log Octanol-Air Partition Coefficient (Log K_{oa})	9.63	Calculated using EPI Suite
8	Soil Adsorption Coefficient (Log K_{OC})	2.48	Calculated using EPI Suite
9	Enthalpy of Vaporization (kJ/mol)	61.50	Advanced Chemistry Development Lab Inc. Database.
10	Energy of Highest Occupied Molecular Orbital (eV)	-6.29	Calculated using MOPAC
11	Energy of Lowest Unoccupied Molecular Orbital (eV)	0.19	Calculated using MOPAC

4.2 Biodegradation, Oxidation and Hydrolysis Rate Constants of Chemicals

In this section values for biodegradation, oxidation and hydrolysis rate constant are presented in tables 12, 13 and 14 respectively. The values of the rate constants were extracted from relevant literature (discussed earlier in Chapter 3.) and a brief note of the study made in the literature from which the values were extracted is also presented in the tables. One or more values of biodegradation oxidation and hydrolysis rate constants were available and are recorded in tables 12, 13 and 14 respectively.

Table 13 Biodegradation Rate of chemicals

Chemical Name	Biodegradation Rate	Note		Reference
Geosmin	0.25 d^{-1}	Initial Concentration of 100 ng/L	The degradation of geosmin was in presence of single gram negative bacteria. (The degradation was at 22^0C). Pseudo first order reaction rate.	Hoefel et al. (2009)
Gesomin	0.58 d^{-1}	Initial Concentration of 500 ng/L		
Gesomin	0.67 d^{-1}	Initial Concentration of 1000 ng/L		
Geosmin	0.24 d^{-1}	Initial concentration 200 ng/L	The degradation was in sand filters of the water treatment plant. Pseudo first order reaction rate.	Ho et al. (2007)
Geosmin	0.21 d^{-1}	Initial concentration 50 ng/L		
Geosmin	0.120 d^{-1}	Initial concentration 200 ng/L		
2-MIB	0.18 d^{-1}	Initial concentration 200 ng/L	The degradation was in sand filters of the water treatment plant. Pseudo first order reaction rate.	Ho et al. (2007)
2-MIB	0.14 d^{-1}	Initial concentration 50 ng/L		
2-MIB	0.10 d^{-1}	Initial concentration 200 ng/L		
2,4-Dichlorophenol	0.06 d^{-1}	Nitrogen source NH_4Cl	The degradation by consortium of Bacillus species.	Herrera (2008)
2,4-Dichlorophenol	0.09 d^{-1}	Nitrogen source $KMNO_2$		
2,4-Dichlorophenol	0.01-0.9 d^{-1}	Degradation in aerobic aquifer	First order rate of reaction.	Nielsen et al. (1996)
2, 4-Dichlorophenol	0.48 d^{-1}	Addition of glucose as carbon source	First order rate of reaction.	Ziagova et al. (2006)
Acetaminophen	0.393 d^{-1}	Enzyme reaction	First order rate of reaction	Lu et al. (2009)
Triclosan	0.19-0.28 d^{-1}	CO_2 evolution	First order rate of reaction.	Hansveit et al. (2003)
Atrazine	0.9264 d^{-1}	Degradation in fixed-film sand column	First order rate of reaction.	Crawford et al. (2000)

Table 14 Oxidation rates of chemicals

Chemical Name	Oxidation Rate	Note		Reference
Geosmin	0.0633 min^{-1}	Using Titanium dioxide photocatalyst	Pseudo first order reaction rate.	Lawton (2003)
Geosmin	5-11 $M^{-1}s^{-1}$	Ozonation	Second order rate constants	Westerhoff et al. (2006)
Geosmin	0.10 $M^{-1}s^{-1}$	Ozonation	Second order rate constants	Peter et al. (2007)
2-MIB	0.1979 min^{-1}	Using Titanium dioxide photocatalyst	Pseudo first order reaction rate.	Lawton (2003)
2-MIB	4-9 $M^{-1}s^{-1}$	Ozonation	Second order rate constants	Westerhoff et al. (2006)
2-MIB	0.35 $M^{-1}s^{-1}$	Ozonation	Second order rate constants	Peter et al. (2007)
2, 4 Dichlorophenol	6.085×10^{8} $M^{-1}s^{-1}$	Ozonation	First order rate of reaction	Benitez et al. (2000)
Triclosan	3.8×10^{8} $M^{-1}s^{-1}$	Ozonation	Second order rate of reaction.	Suarez et al. (2007)
Atrazine	3×10^{-3} $M^{-1}s^{-1}$	Ozonation	First order rate of reaction	Hoigne and Bader (1983)
Acetaminophen	1.41×10^{3} $M^{-1}s^{-1}$	Ozonation	Second order rate of reaction	Andreozzi et al. (2003)

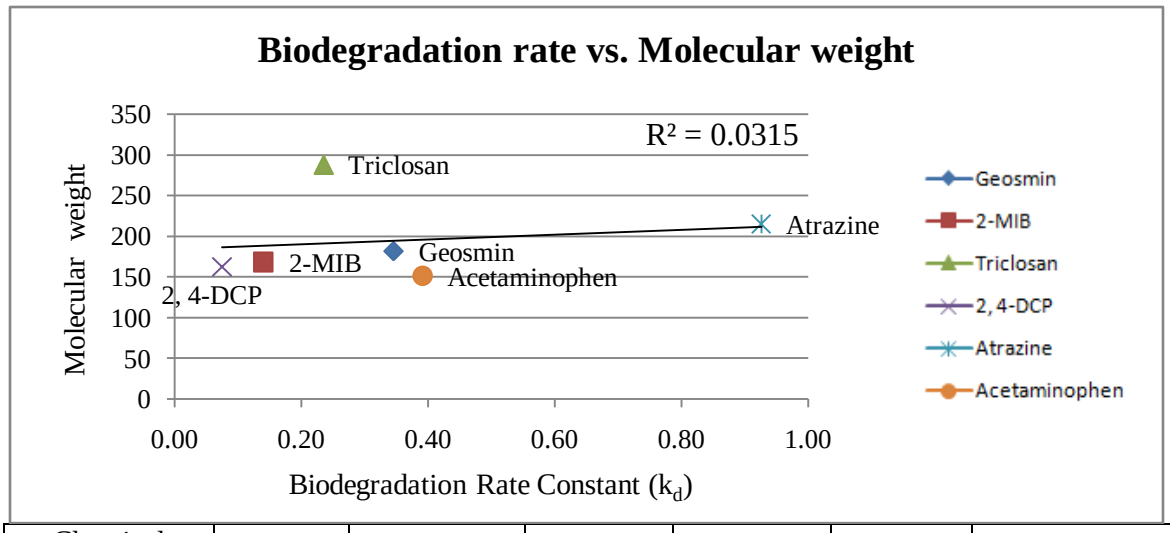
Table 15 Hydroxyl Reaction Rate

Chemical Name	Oxidation Rate	Note		Reference
Geosmin	$7.80\times10^{9} M^{-1}s^{-1}$	UV/H_2O_2	Second order reaction rate.	Peter et al. (2007)
Geosmin	0.12 min^{-1}	Ultrasonic irradication	First order rate constants	Song et al. (2007)
Geosmin	$9.5\times10^{9} M^{-1}s^{-1}$	Oxidation process/ H_2O_2	Second order rate constants	Westerhoff et al. (2006)
2-MIB	0.070 min^{-1}	Ultrasonic irradication	First order rate constants	Song et al. (2007)
2-MIB	$8.2\times10^{9} M^{-1}s^{-1}$	Oxidation process/ H_2O_2	Second order rate constants	Westerhoff et al. (2006)
2-MIB	$5.09\times10^{9} M^{-1}s^{-1}$	UV/H_2O_2	Second order reaction rate.	Peter et al. (2007)
2,4-Dichlorophenol	7×10^{-4} min^{-1}	Sono Fenton Method	First order rate constant.	Lee et al. (2005)
2,4-Dichlorophenol	0.057 min^{-1}	Advanced Oxidation Process	First order rate constant.	Momami et al. (2003)
Triclosan	$5.4\times10^{9} M^{-1}s^{-1}$	Reaction with hydroxyl radicals	Second order rate of reaction.	Latch et. al(2005); Arnold et al.(2003)
Atrazine	$7.3\times10^{8} M^{-1}s^{-1}$	Reaction with hydroxyl radicals	First order rate of reaction.	Scholles and Willson (1967)
Acetaminophen	$1.7\times10^{9} M^{-1}s^{-1}$	Reaction with hydroxyl radicals	Second order rate of reaction	Yang et al. (2009)

In table 15, the data used in the study is summarized. In cases for compounds in which the values of rate constants were more than one, average values were used and these are presented in table 15. Following this table 15, are the graphs which were made for finding the correlations between descriptors and rate constants based on the R^2 value calculated from the graphs. Graphs of biodegradation rate constants were first plotted against the descriptors first (figures 4 to 13), followed by oxidation rate constant (figures 14 to 22) and hydrolysis rate constants (figures 23-32) respectively.

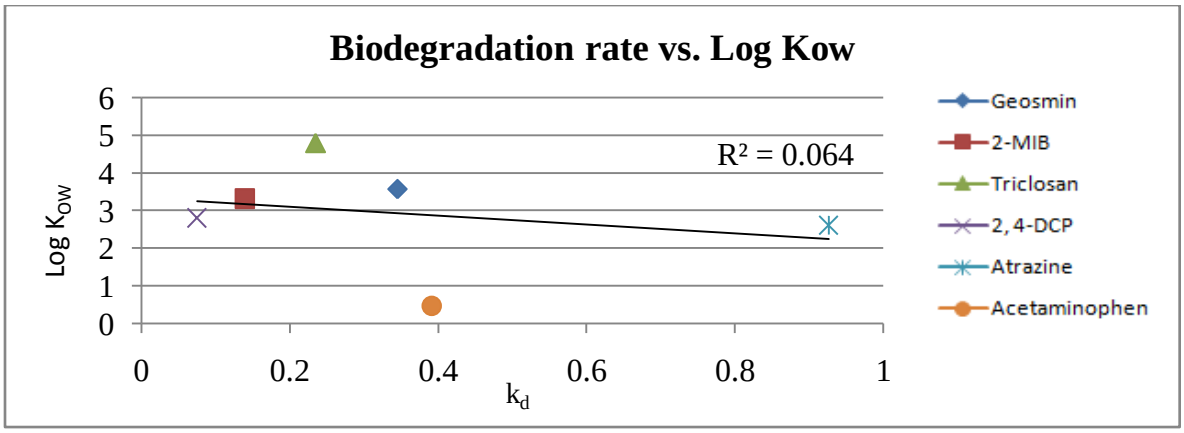
Table 16 Summary of data

Properties	Chemicals					
	Geosmin	2-MIB	Triclosan	2,4 DCP	Atrazine	Acetaminophen
Molecular Weight (Da)	182	168	288	162	215	151
Log Kow	3.57	3.31	4.80	2.80	2.60	0.46
Water Solubility (mg/L)	157.00	194.50	10.00	4500.00	34.70	1.29×10^{4}
Henry's Law Constant (atm-m^3/mole, 25^0C)	2.30×10^{-3}	2.70×10^{-3}	6.15×10^{-6}	1.00×10^{-4}	1.21×10^{-7}	2.63×10^{-11}
Log Koa	6.88	6.75	11.45	7.70	9.63	11.04
Log Koc	2.48	2.35	3.93	2.79	2.48	1.32
Enthalpy of Vaporization (kJ/mol)	59.00	51.80	61.20	46.50	61.50	66.20
Vapor Pressure(mm of Hg, 25^0C)	5.49×10^{-5}	55.1×10^{-3}	3.26×10^{-5}	12×10^{-2}	2.89×10^{-7}	1.43×10^{-7}
E_{LUMO} (eV)	2.96	2.32	0.52	0.82	0.19	-0.49
E_{HOMO} (eV)	-10.46	-9.17	-5.62	-6.49	-6.29	-5.53
Biodegradati--on Rate (per day)	0.35	0.14	0.24	0.07	0.93	0.39
Oxidation Rate (per mole sec)	8.00	6.50	3.80×10^{7}	6.09×10^{8}	4.50	3×10^{-3}
Hydrolysis Rate (per mole sec)	9.50×10^{9}	8.20×10^{9}	7.30×10^{9}	7.20×10^{9}	2.70×10^{9}	1.7×10^{9}



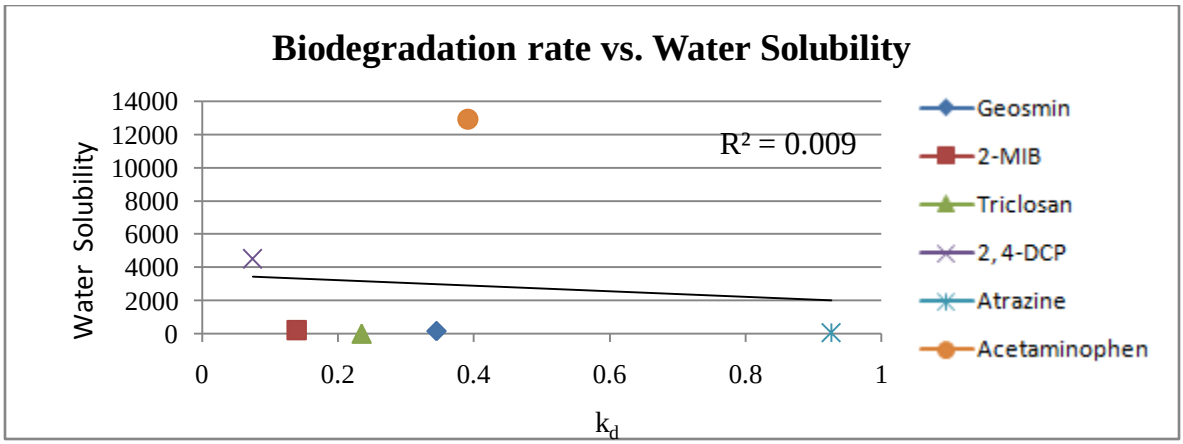
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Molecular weight (Da)	182.00	168.00	288.00	162.00	215.00	151.00
Biodegradation Rate (per day)	0.35	0.14	0.24	0.08	0.93	0.39

Figure 7 Biodegradation rate vs. Molecular weight



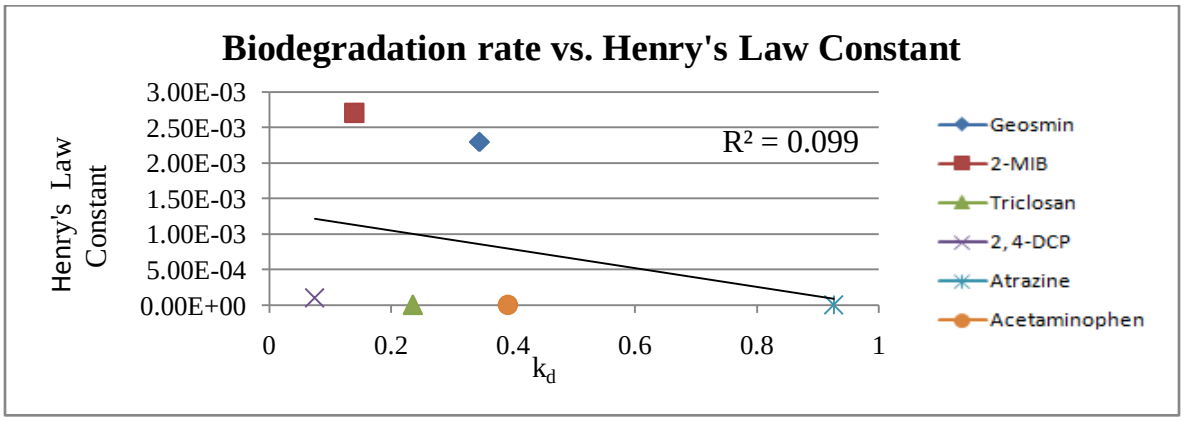
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Log Kow	3.57	3.31	4.8	2.8	2.6	0.46
Biodegradation Rate (per day)	0.35	0.14	0.24	0.08	0.93	0.39

Figure 8 Biodegradation rate vs. Log K_{OW}



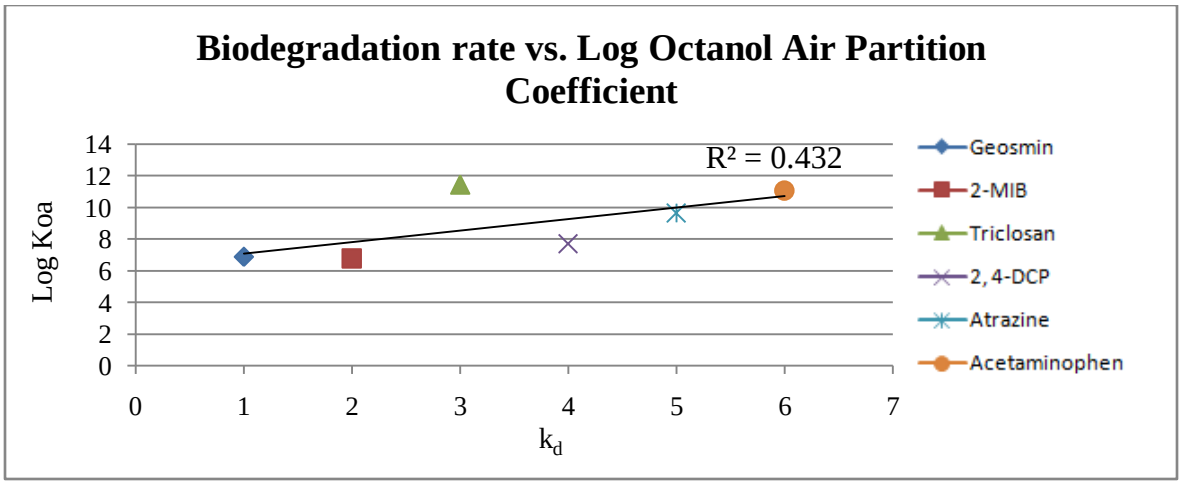
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Water Solubility (mg/L)	157.00	194.50	10.00	4500.00	34.70	1.29×10^{4}
Biodegradation Rate (per day)	0.35	0.14	0.24	0.08	0.93	0.39

Figure 9 Biodegradation rate vs. Water Solubility



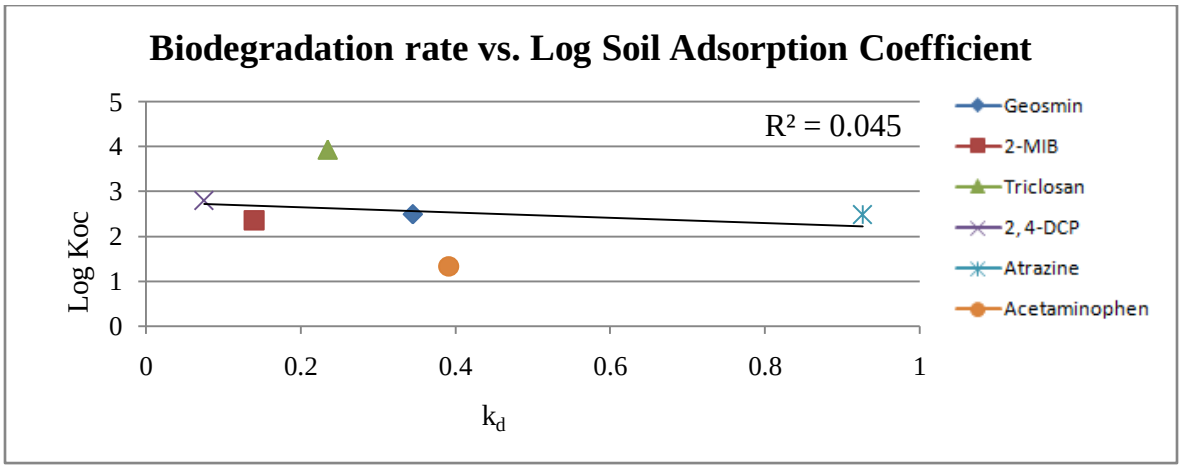
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Henry's Law Constant (atm-m^3/mole, 25^0C)	2.30×10^{-3}	2.70×10^{-3}	6.15×10^{-6}	1.00×10^{-4}	1.21×10^{-7}	2.63×10^{-11}
Biodegradation Rate (per day)	0.35	0.14	0.24	0.08	0.93	0.39

Figure 10 Biodegradation rate vs. Henry's Law Constant



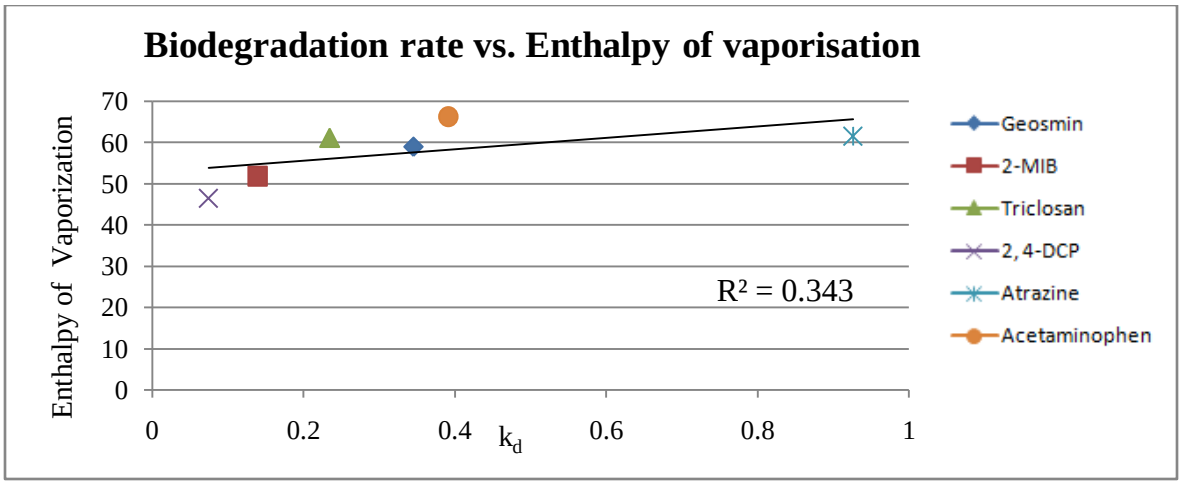
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Log Koa	6.88	6.75	11.45	7.70	9.63	11.04
Biodegradation Rate (per day)	0.35	0.14	0.24	0.08	0.93	0.39

Figure 11 Biodegradation rate vs. Log Octanol Air Partition Coefficient



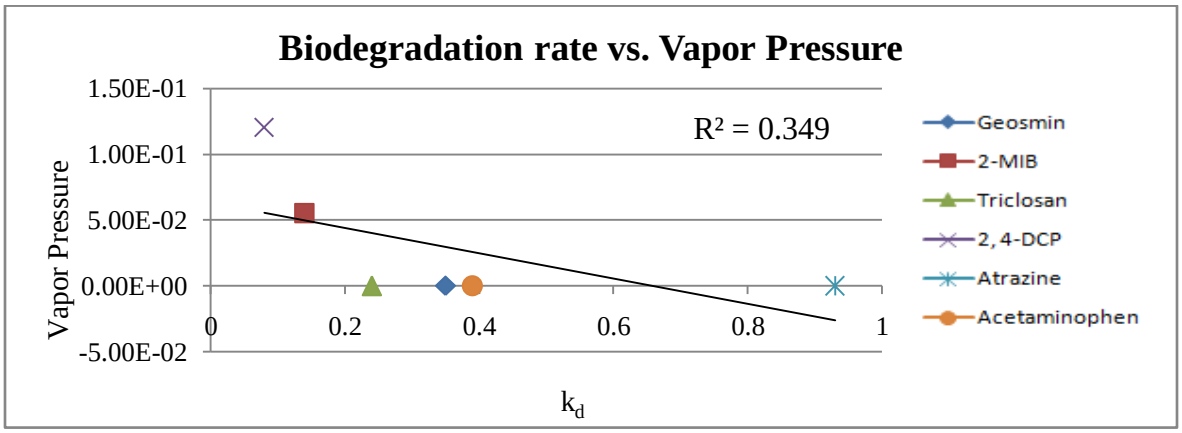
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Log Koc	2.48	2.35	3.93	2.79	2.48	1.32
Biodegradation Rate (per day)	0.35	0.14	0.24	0.08	0.93	0.39

Figure 12 Biodegradation rate vs. Soil Adsorption Coefficient



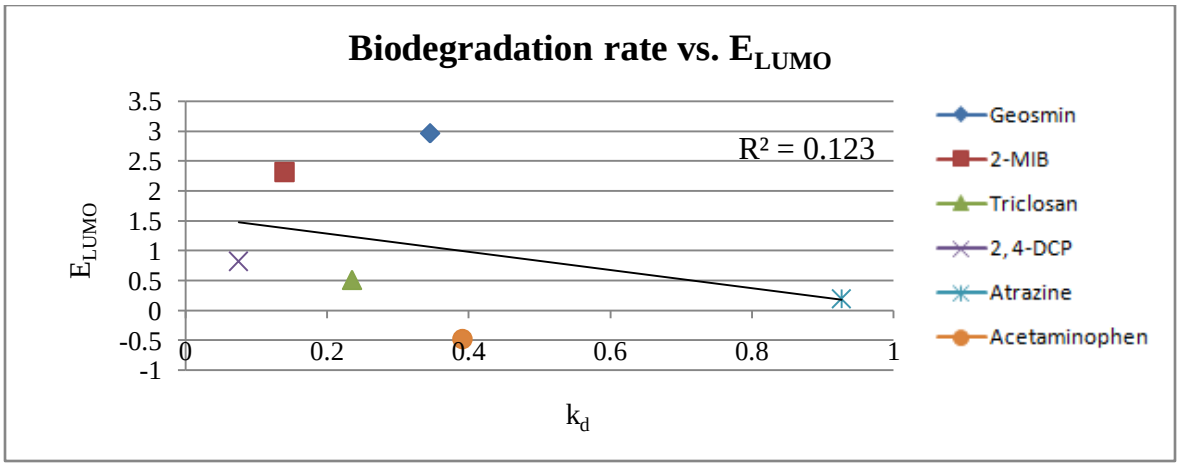
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Enthalpy of Vaporization (kJ/mol)	59.00	51.80	61.20	46.50	61.50	66.20
Biodegradation Rate (per day)	0.35	0.14	0.24	0.08	0.93	0.39

Figure 13 Biodegradation rate vs. Enthalpy of vaporization



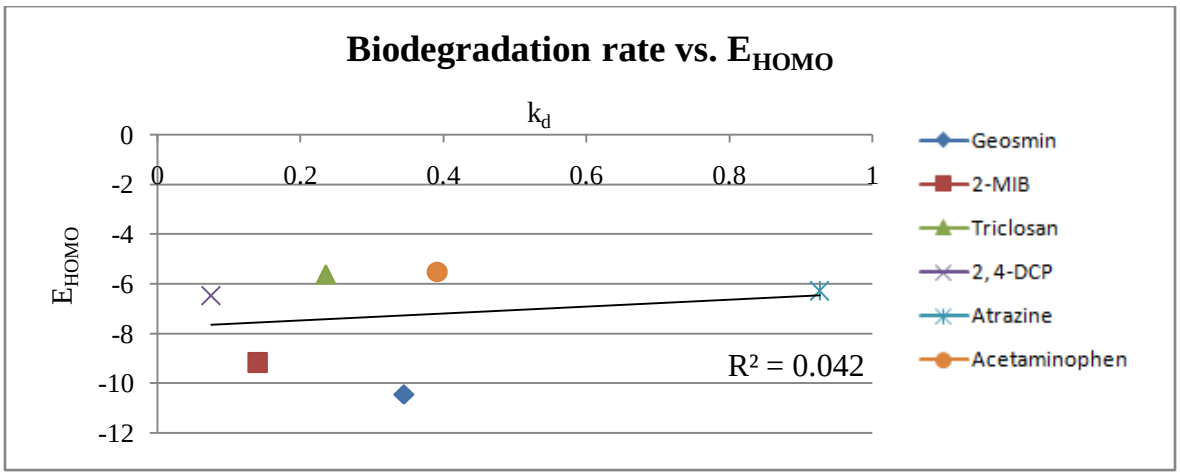
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Vapor Pressure(mm of Hg, 25^0C)	5.49×10^{-5}	55.1×10^{-3}	3.26×10^{-5}	12×10^{-2}	2.89×10^{-7}	1.43×10^{-7}
Biodegradation Rate (per day)	0.35	0.14	0.24	0.08	0.93	0.39

Figure 14 Biodegradation rate vs. Vapor Pressure



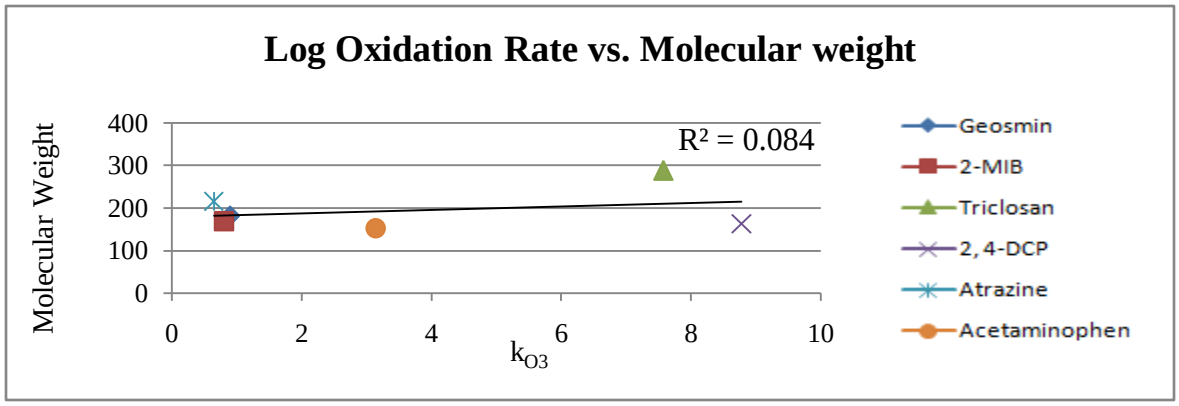
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
E_{LUMO} (eV)	2.96	2.32	0.52	0.82	0.19	-0.49
Biodegradation Rate (per day)	0.35	0.14	0.24	0.08	0.93	0.39

Figure 15 Biodegradation rate vs. E_{LUMO}



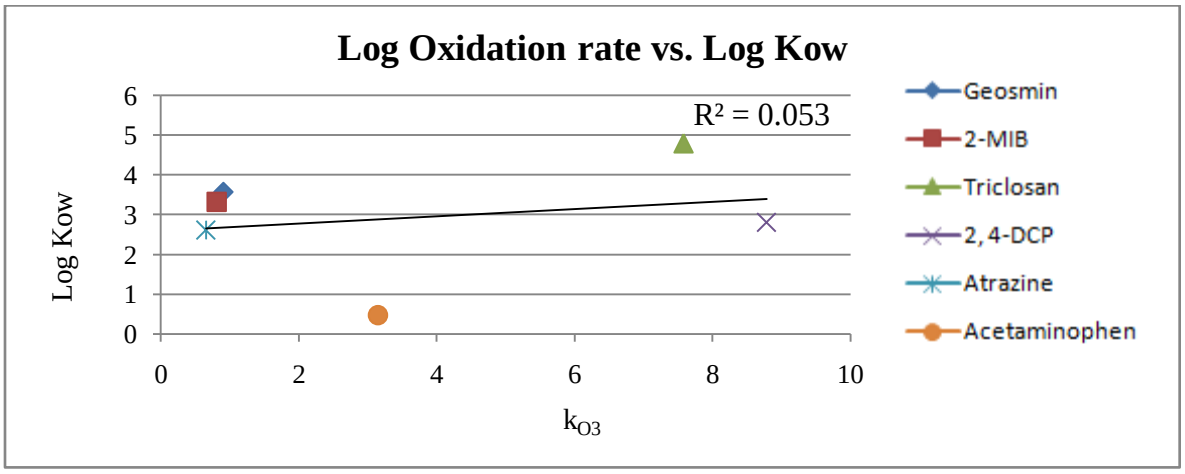
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
E_{HOMO} (eV)	-10.46	-9.17	-5.62	-6.49	-6.29	-5.53
Biodegradation Rate (per day)	0.35	0.14	0.24	0.08	0.93	0.39

Figure 16 Biodegradation rate vs. E_{HOMO}



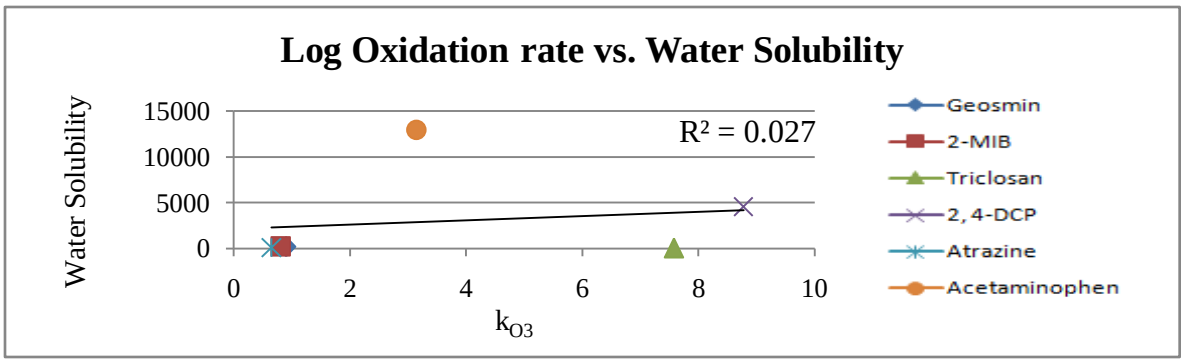
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Molecular weight (Da)	182.00	168.00	288.00	162.00	215.00	151.00
Log Oxidation Rate (per mole sec)	0.90	0.81	7.58	8.78	0.65	3.15

Figure 17 Log Oxidation rate vs. Molecular weight



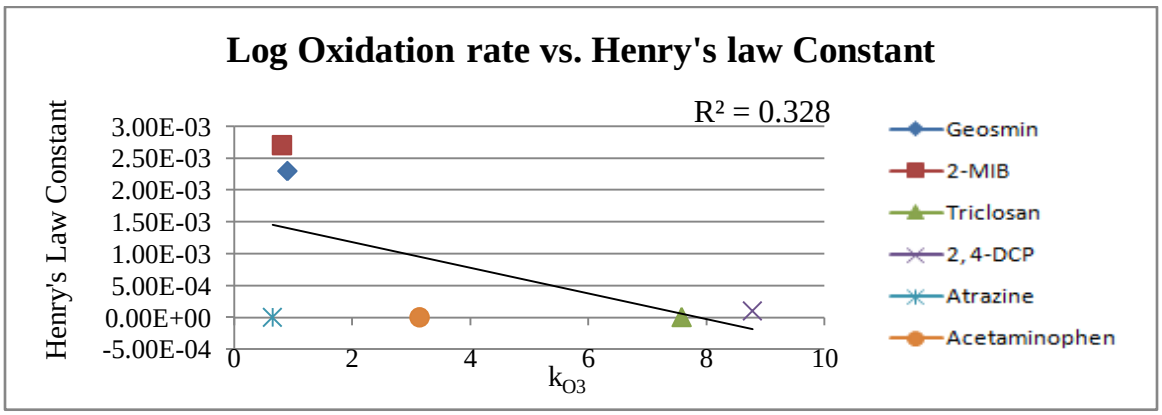
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Log Kow	3.57	3.31	4.8	2.8	2.6	0.46
Log Oxidation Rate (per mole sec)	0.90	0.81	7.58	8.78	0.65	3.15

Figure 18 Log Oxidation rate vs. Log K_{OW}



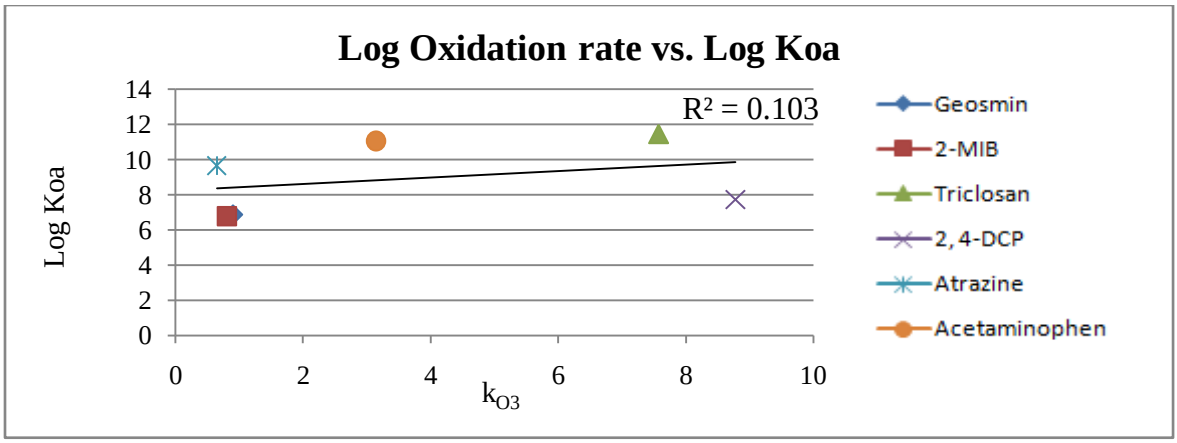
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Water Solubility (mg/L)	157.00	194.50	10.00	4500.00	34.70	1.29×104
Log Oxidation Rate (per mole sec)	0.90	0.81	7.58	8.78	0.65	3.15

Figure 19 Log Oxidation rate vs. Water Solubility



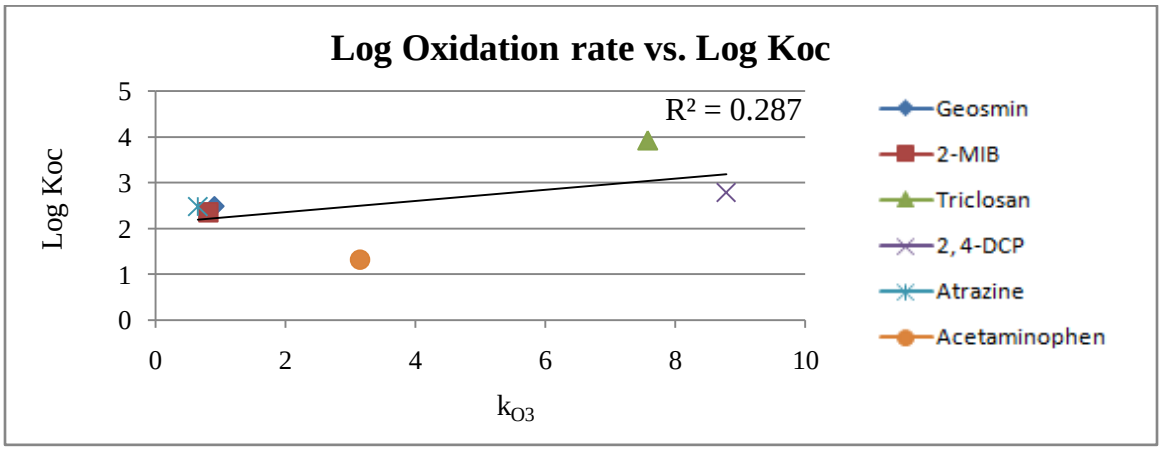
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Henry's Law Constant (atm-m^3/mole, 25^0C)	2.30×10^{-3}	2.70×10^{-3}	6.15×10^{-6}	1.00×10^{-4}	1.21×10^{-7}	2.63×10^{-11}
Log Oxidation Rate (per mole sec)	0.90	0.81	7.58	8.78	0.65	3.15

Figure 20 Log Oxidation rate vs. Henry's Law Constant



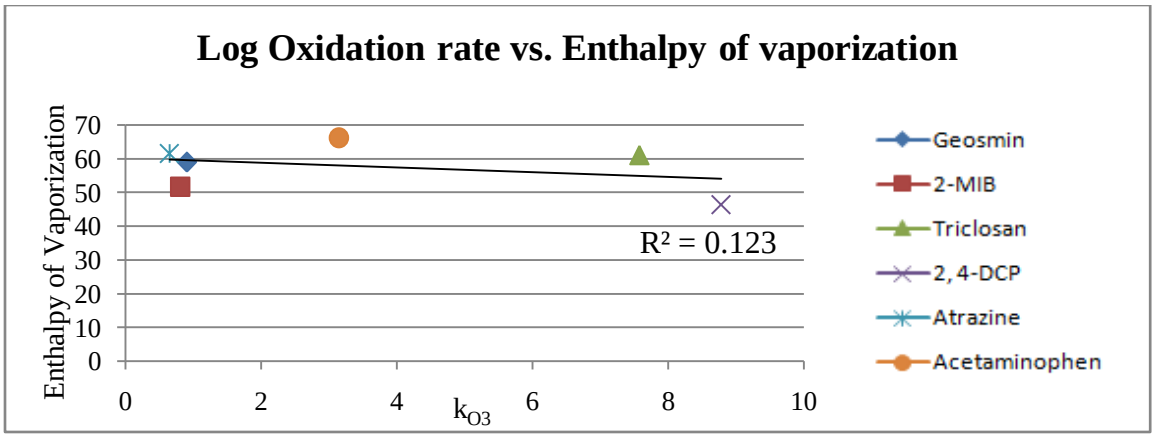
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Log Koa	6.88	6.75	11.45	7.70	9.63	11.04
Log Oxidation Rate (per mole sec)	0.90	0.81	7.58	8.78	0.65	3.15

Figure 21 Log Oxidation rate vs. Log Octanol air partition coefficient (Log Koa)



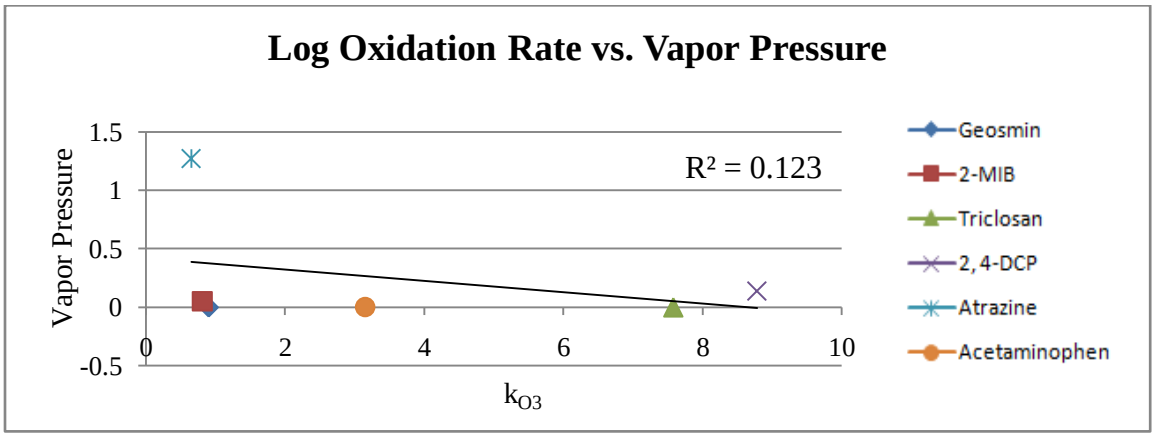
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Log Koc	2.48	2.35	3.93	2.79	2.48	1.32
Log Oxidation Rate (per mole sec)	0.90	0.81	7.58	8.78	0.65	3.15

Figure 22 Log Oxidation rate vs. Soil Adsorption Coefficient



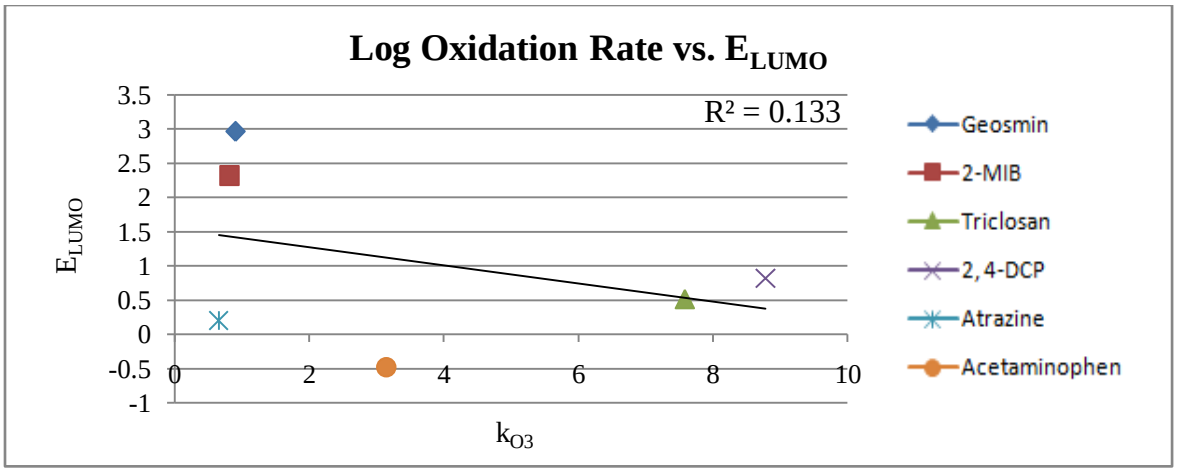
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Enthalpy of Vaporization (kJ/mol)	59.00	51.80	61.20	46.50	61.50	66.20
Log Oxidation Rate (per mole sec)	0.90	0.81	7.58	8.78	0.65	3.15

Figure 23 Log Oxidation rate vs. Enthalpy of vaporization



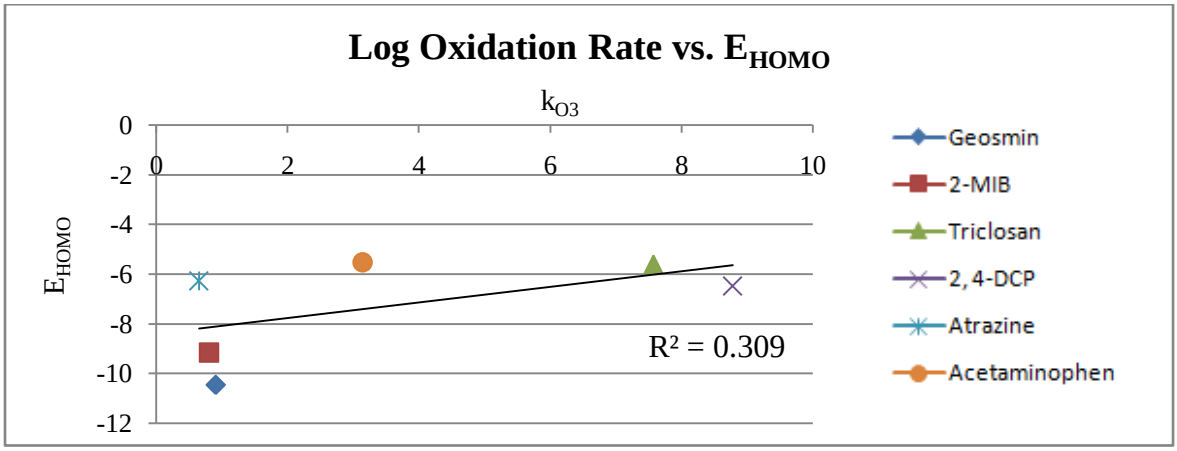
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Vapor Pressure(mm of Hg, 25^0C)	5.49×10^{-5}	55.1×10^{-3}	3.26×10^{-5}	12×10^{-2}	2.89×10^{-7}	1.43×10^{-7}
Log Oxidation Rate (per mole sec)	0.90	0.81	7.58	8.78	0.65	3.15

Figure 24 Log Oxidation rate vs. Vapor Pressure



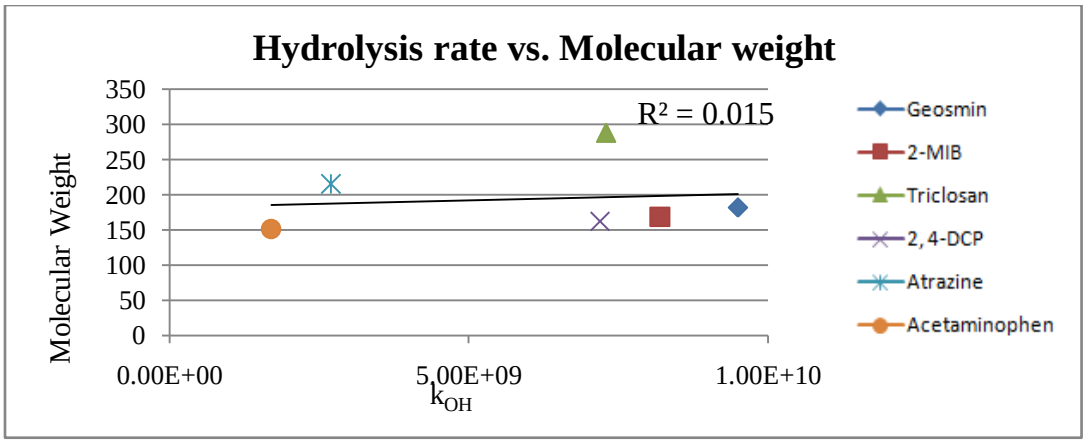
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
E_{LUMO} (eV)	2.96	2.32	0.52	0.82	0.19	-0.49
Log Oxidation Rate (per mole sec)	0.90	0.81	7.58	8.78	0.65	3.15

Figure 25 Log Oxidation rate vs. E_{LUMO}



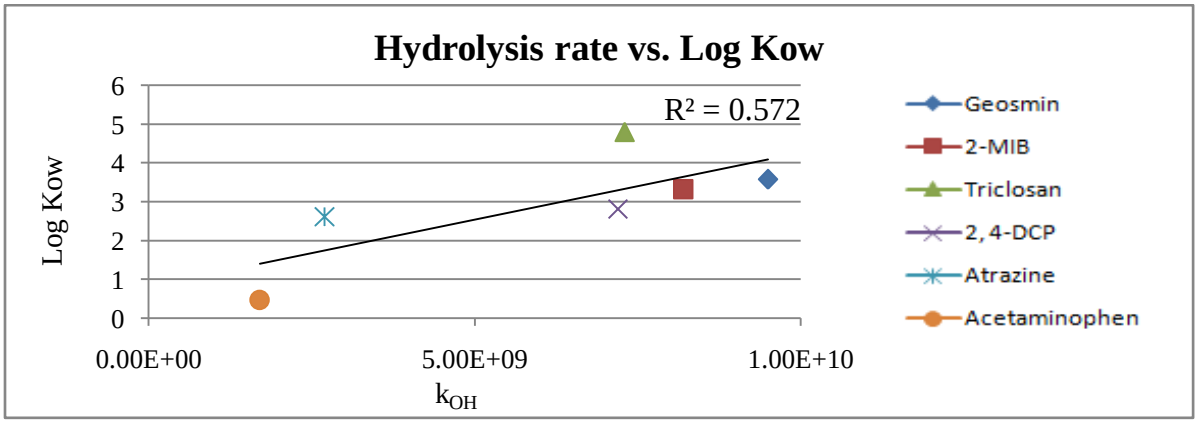
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
E_{HOMO} (eV)	-10.46	-9.17	-5.62	-6.49	-6.29	-5.53
Log Oxidation Rate (per mole sec)	0.90	0.81	7.58	8.78	0.65	3.15

Figure 26 Log Oxidation rate vs. E_{HOMO}



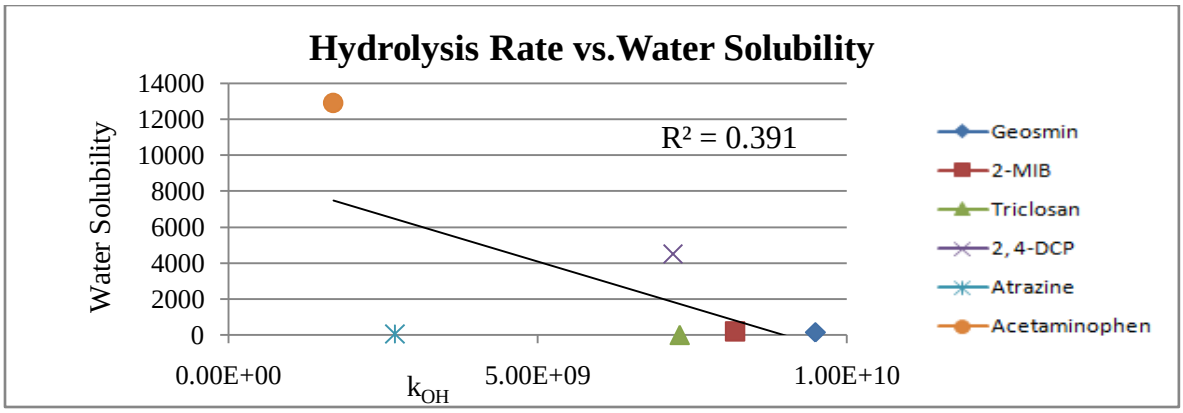
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Molecular weight (Da)	182.00	168.00	288.00	162.00	215.00	151.00
Hydrolysis Rate (per mole sec)	9.50×10^{9}	8.20×10^{9}	7.30×10^{9}	7.20×10^{9}	2.70×10^{9}	1.70×10^{9}

Figure 27 Hydrolysis rate vs. Molecular weight



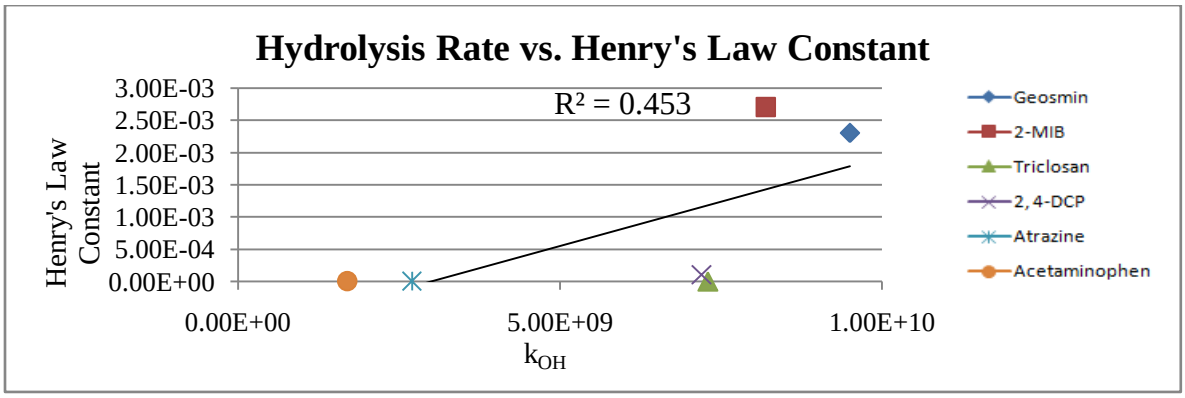
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Log Kow	3.57	3.31	4.8	2.8	2.6	0.46
Hydrolysis Rate (per mole sec)	9.50×10^{9}	8.20×10^{9}	7.30×10^{9}	7.20×10^{9}	2.70×10^{9}	1.70×10^{9}

Figure 28 Hydrolysis rate vs. Log K_{OW}



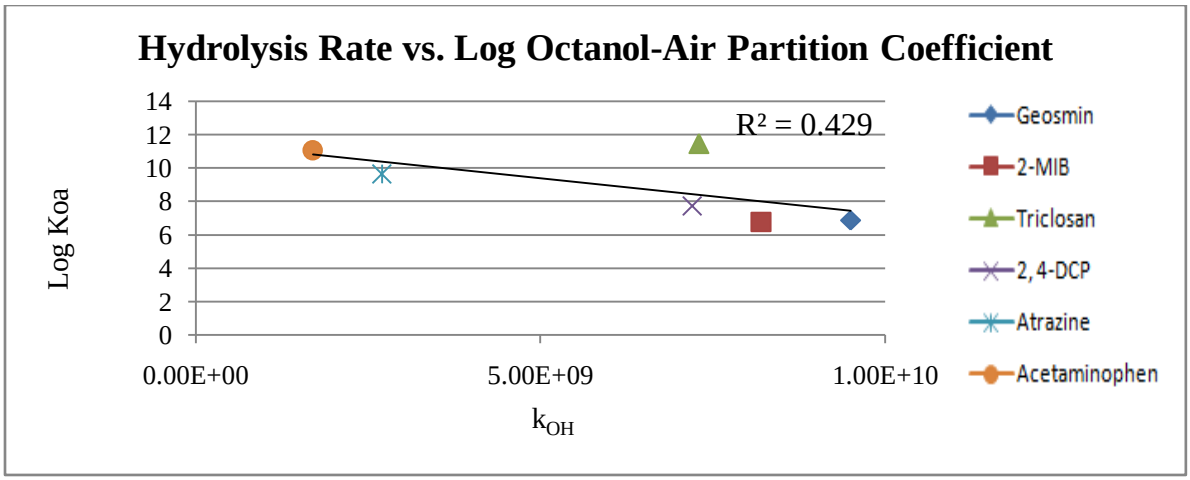
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Water Solubility (mg/L)	157.00	194.50	10.00	4500.00	34.70	1.29×10^{4}
Hydrolysis Rate (per mole sec)	9.50×10^{9}	8.20×10^{9}	7.30×10^{9}	7.20×10^{9}	2.70×10^{9}	1.70×10^{9}

Figure 29 Hydrolysis rate vs. Water Solubility



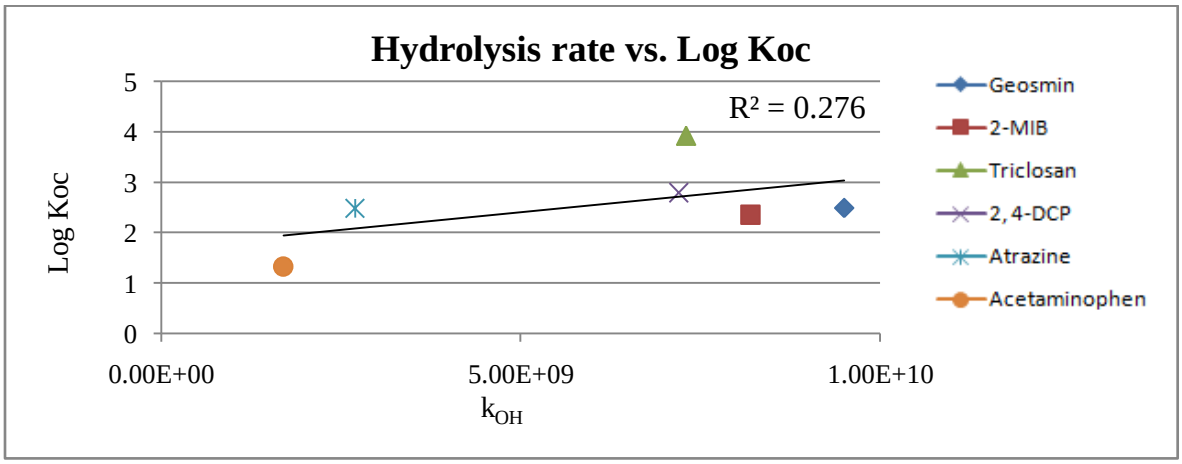
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Henry's Law Constant (atm-m^3/mole, 25^0C)	2.30×10^{-3}	2.70×10^{-3}	6.15×10^{-6}	1.00×10^{-4}	1.21×10^{-7}	2.63×10^{-11}
Hydrolysis Rate (per mole sec)	9.50×10^{9}	8.20×10^{9}	7.30×10^{9}	7.20×10^{9}	2.70×10^{9}	1.70×10^{9}

Figure 30 Hydrolysis rate vs. Henry's Law Constant



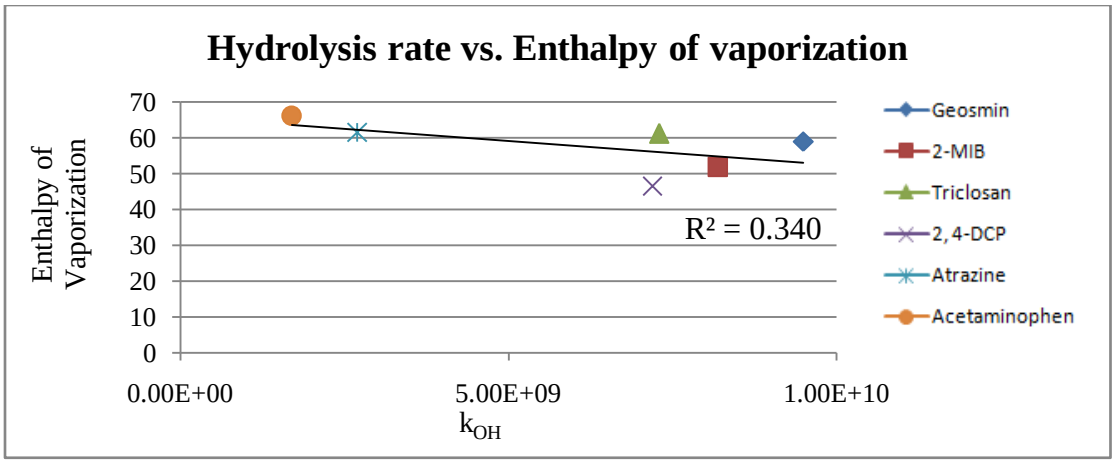
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Log Koa	6.88	6.75	11.45	7.70	9.63	11.04
Hydrolysis Rate (per mole sec)	9.50×10^{9}	8.20×10^{9}	7.30×10^{9}	7.20×10^{9}	2.70×10^{9}	1.70×10^{9}

Figure 31 Hydrolysis rate vs. Log Octanol Air Partition Coefficient



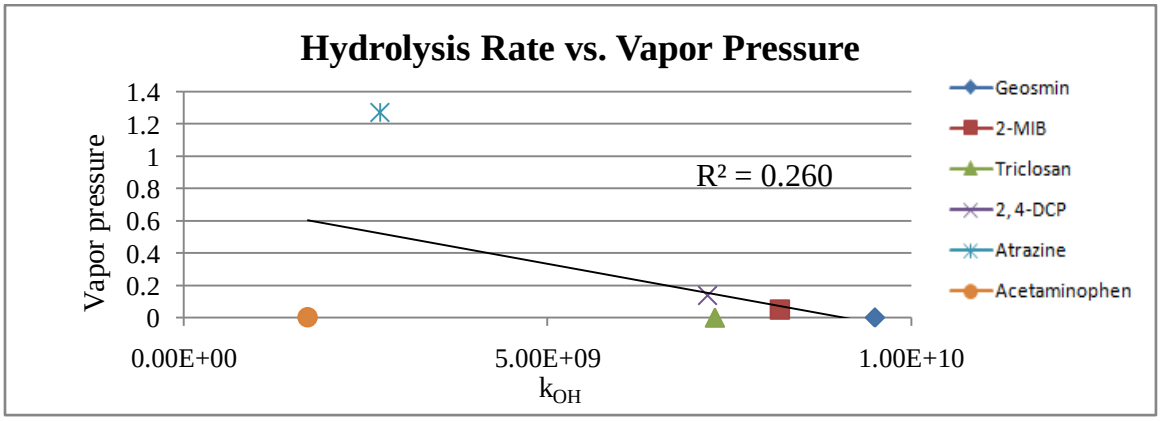
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Log Koc	2.48	2.35	3.93	2.79	2.48	1.32
Hydrolysis Rate (per mole sec)	9.50×10^{9}	8.20×10^{9}	7.30×10^{9}	7.20×10^{9}	2.70×10^{9}	1.70×10^{9}

Figure 32 Hydrolysis rate vs. Soil Adsorption coefficient



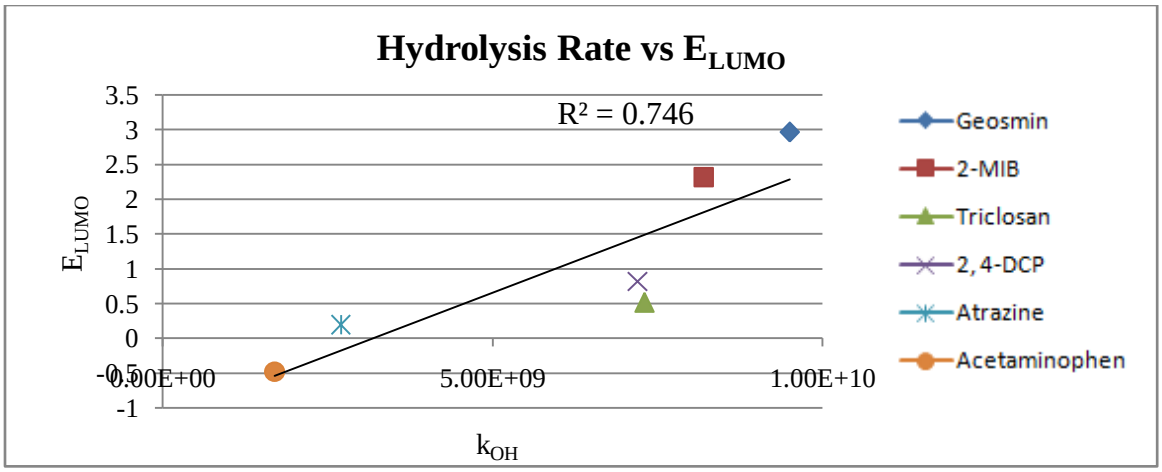
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Enthalpy of Vaporization (kJ/mol)	59.00	51.80	61.20	46.50	61.50	66.20
Hydrolysis Rate (per mole sec)	9.50×10^{9}	8.20×10^{9}	7.30×10^{9}	7.20×10^{9}	2.70×10^{9}	1.70×10^{9}

Figure 33 Hydrolysis rate vs. Enthalpy of vaporization



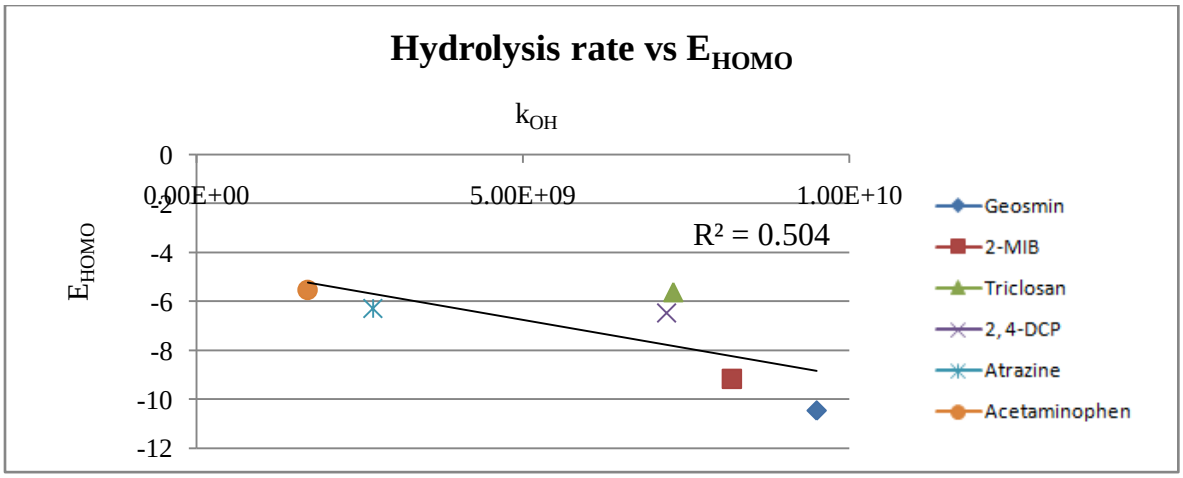
Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
Vapor Pressure(mm of Hg, 25^{0}C)	5.49×10^{-5}	55.1×10^{-3}	3.26×10^{-5}	12×10^{-2}	2.89×10^{-7}	1.43×10^{-7}
Hydrolysis Rate (per mole sec)	9.50×10^{9}	8.20×10^{9}	7.30×10^{9}	7.20×10^{9}	2.70×10^{9}	1.70×10^{9}

Figure 34 Hydrolysis rate vs. Vapor Pressure



Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
E_{LUMO} (eV)	2.96	2.32	0.52	0.82	0.19	-0.49
Hydrolysis Rate (per mole sec)	9.50×10^{9}	8.20×10^{9}	7.30×10^{9}	7.20×10^{9}	2.70×10^{9}	1.70×10^{9}

Figure 35 Hydrolysis rate vs. E_{LUMO}



Chemical Name	Geosmin	2-MIB	Triclosan	2, 4-DCP	Atrazine	Acetaminophen
E_{HOMO} (eV)	-10.46	-9.17	-5.62	-6.49	-6.29	-5.53
Hydrolysis Rate (per mole sec)	9.50×10^{9}	8.20×10^{9}	7.30×10^{9}	7.20×10^{9}	2.70×10^{9}	1.70×10^{9}

Figure 36 Hydrolysis rate vs. E_{HOMO}

4.3 Discussion

In this study an attempt was made to correlate the descriptors (physical-chemical properties) of geosmin, 2-MIB, 2,4-dichlorophenol, acetaminophen, atrazine and triclosan with activity rates (biodegradation rate, oxidation rate and hydrolysis rate). In this effort, data commonly used was extracted from available literature and in some cases calculated using computational chemistry software. For most of the data analyzed no significant correlations were obtained between the physical-chemical properties and activity rates (biodegradation rate, oxidation rate and hydrolysis rate). One of the reasons may be attributed to studies made in finding the various rate constants from which the data was extracted. All degradation rate constants were extracted from literature for which the study and calculations were not done under same conditions. Also the compounds used are from heterologous groups. Published correlations that are able to predict degradability of compounds displaying varying chemical structure are scarce in comparison to homologous series of compounds (Raymond, et al., 2001). Geosmin and 2-MIB are naturally occurring organic chemicals while the others are produced artificially for commercial use in various industries. Also the purposes for which these chemicals are used are different. Acetaminophen is used as a drug, while triclosan is used for its antimicrobial activity. Atrazine is an herbicide while 2,4-dichlorophenol is an intermediate chemical used for different applications.

Some correlations that showed a potential relationship were obtained between physical-chemical properties of compounds and the three rate constants. The log octanol/air partition coefficient showed some correlation with the biodegradation rate, with an R^2 value of 0.4325. The R^2 value is still low but this may be because the biodegradation rate

constant used were not calculated under identical conditions. The log octanol/air partition coefficient values for compounds were calculated using EPI Suite, so each value was found in a similar manner. The rate of uptake and transport of compound, its binding to the active site of an enzyme, or the rate at which the compound is transformed determines the biodegradation rate of compound. It may be noted that in the absence of a specific uptake mechanism, synthetic organic chemicals are probably transported into bacterial cells by passive diffusion mechanism through the lipid membrane (Parsons and Govers, 1990). As such, a correlation between partitioning in octanol and partitioning in a membrane is not entirely unexpected.

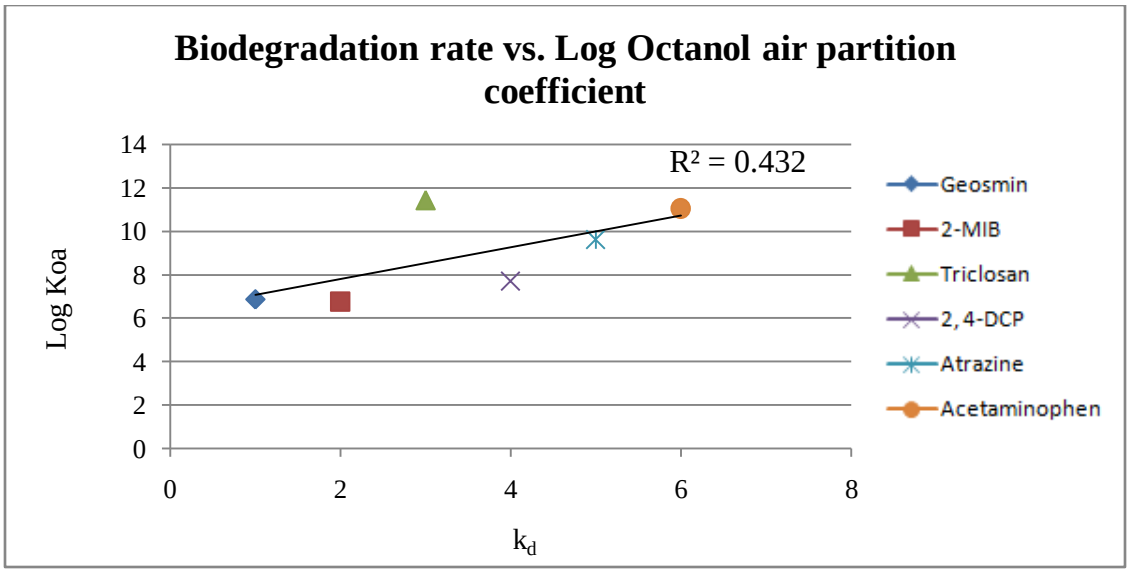


Figure 37 Biodegradation rate constant vs. Log octanol/air partition coefficient.

The enthalpy of vaporization also showed some positive correlation with the biodegradation rate constants with an R^2 value of 0.3431. The R^2 value is still low possibly for the same reasons mentioned above. The rest of the descriptors did not show

any correlations with the biodegradation rate constant, in that most had an R^2 value less than 0.10 for most of the plots.

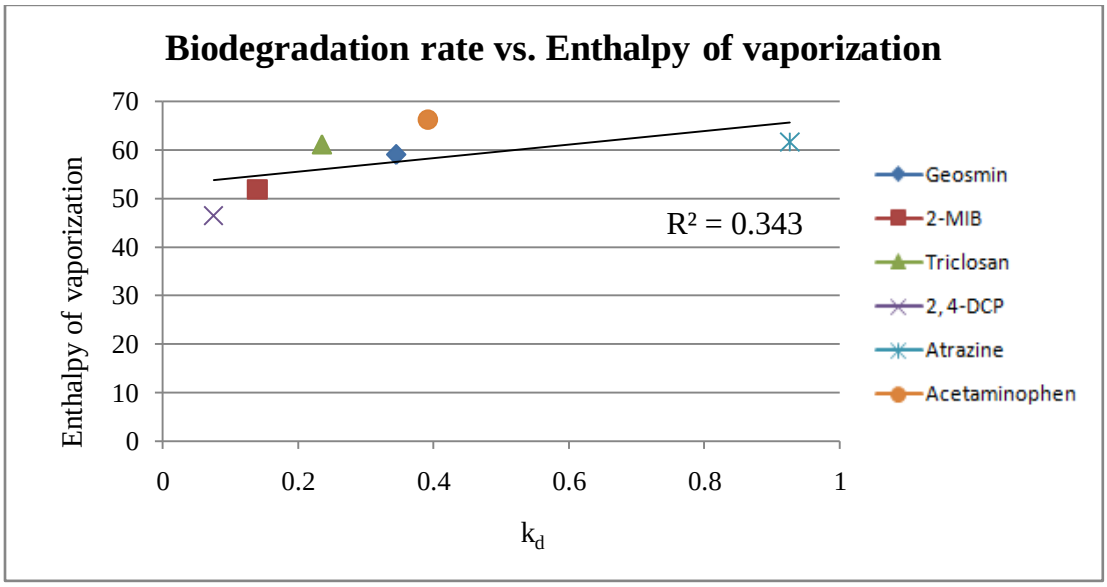


Figure 38 Biodegradation rate vs. Enthalpy of vaporization.

No correlations seemed to exist between the descriptors tested and oxidation rate constants. The oxidation rate constant for the various compounds covered 7 to 8 orders of magnitude. So log of oxidation rate constant was used to plot the graphs, and it appeared to make no significant change in the R^2 value. Similar to biodegradation rate constant the oxidation rate constant extracted from literature were measured under variety of conditions. Most of the correlations, if any can be said to exist, had an R^2 value below 0.20.

The correlation between energy of highest occupied molecular orbital and oxidation rate constant may be explored further. An R^2 value of 0.309 was obtained when energy of highest occupied molecular orbital was plotted against the log of oxidation rate constant. The reasons for this may be that energy of the highest occupied molecular orbital gives a

measure of the energy barrier an electron from the outer electron shell has to overcome to be removed from its orbital. When the reaction mechanism is the same for all compounds, the difference in this energy barrier between different compounds will be rate-determining.

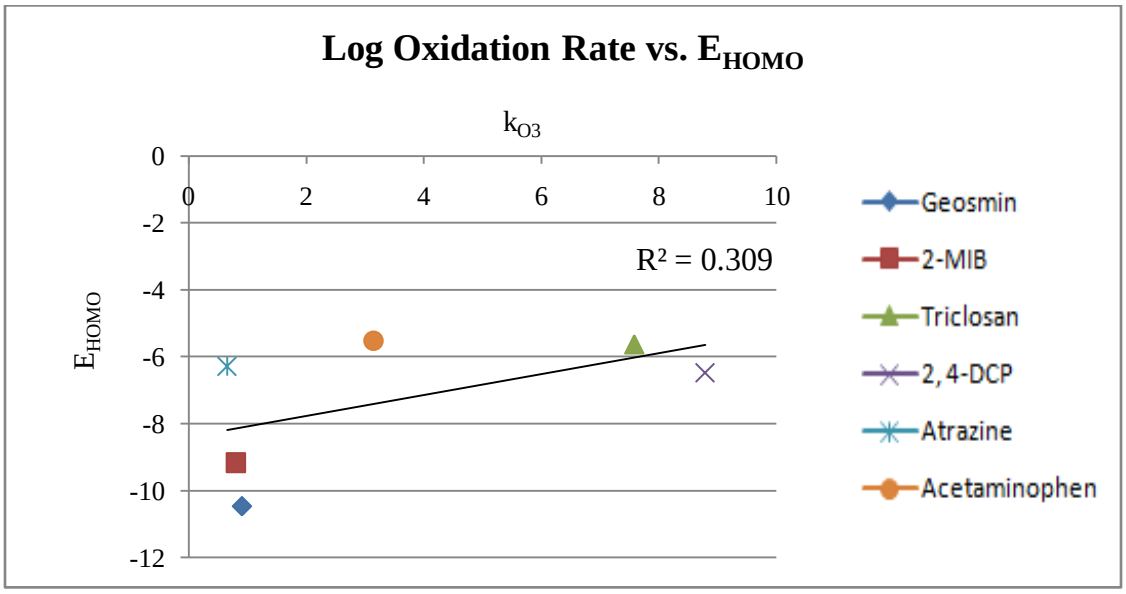


Figure 39 Energy of highest occupied molecular orbital vs. Log oxidation rate.

When the descriptors were plotted against hydrolysis rate most of the plots had low R^2 values as in previous rate constants and may be for the same previous reasons. However an R^2 value of 0.746 and 0.504 was reported when hydrolysis rate was plotted against energy of lowest unoccupied molecular orbital and energy of highest occupied molecular orbit, respectively. Thus a correlation may be said to exist between hydrolysis rate constant and energy of lowest unoccupied molecular orbital (E_{LUMO}). The value of E_{LUMO} and E_{HOMO} can be calculated easily using the MOPAC software and from this an approximate value of hydrolysis rate constant can be predicted saving time and money in calculating the hydrolysis rate constant of other chemicals experimentally.

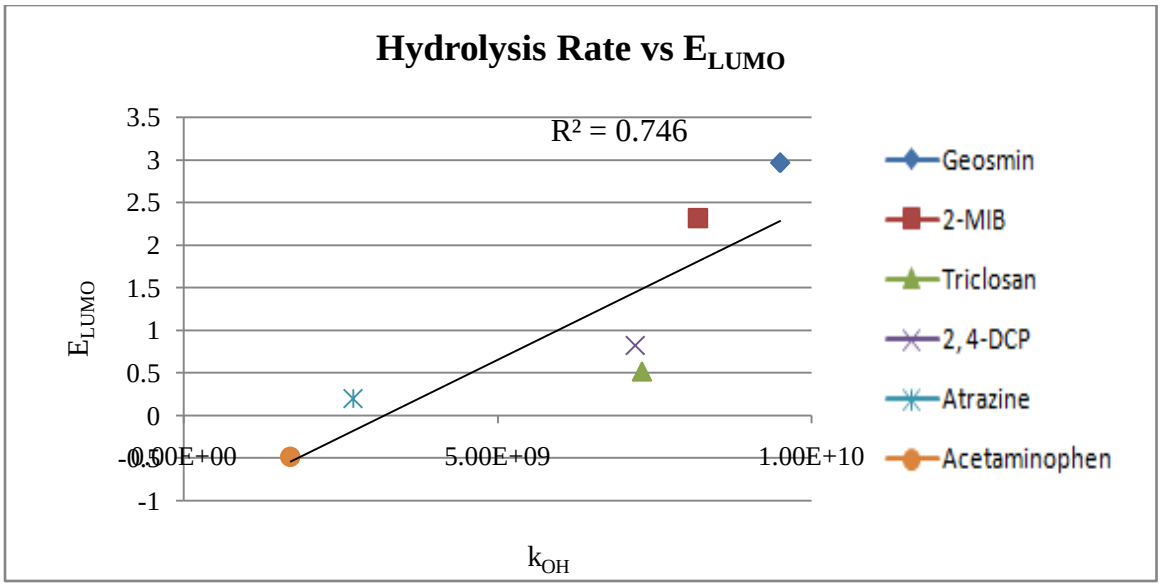


Figure 40 Energy of lowest unoccupied molecular orbital vs. Hydrolysis rate constant.

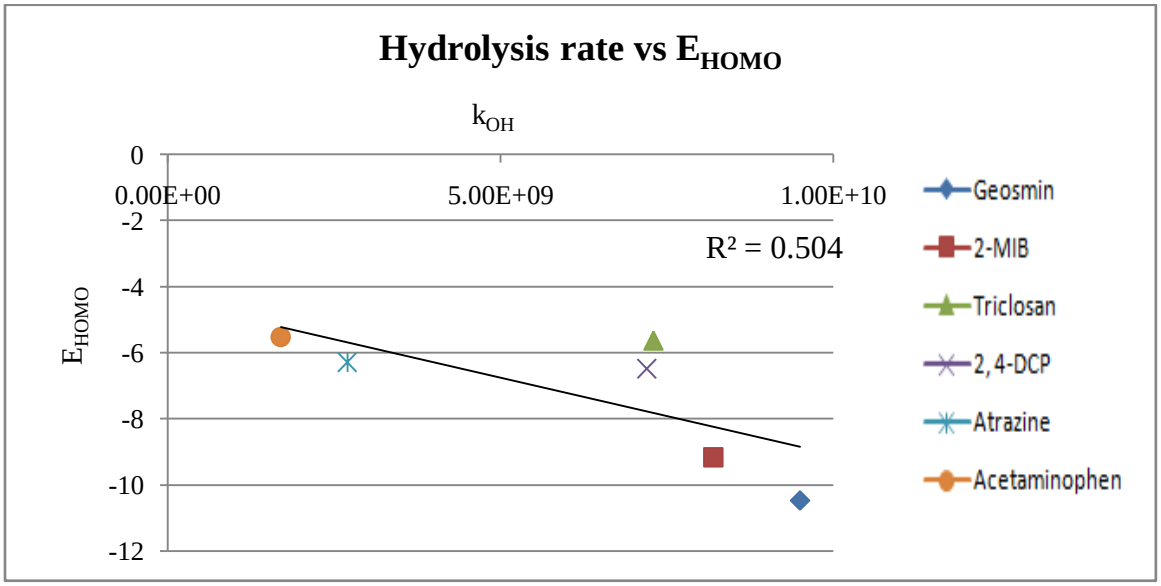


Figure 41 Energy of highest occupied molecular orbital vs. Hydrolysis rate constant.

The hydrolysis rate constant when plotted against log octanol-water partition coefficient, an R^2 value of 0.572 was obtained, indicating a possible correlation between the two.

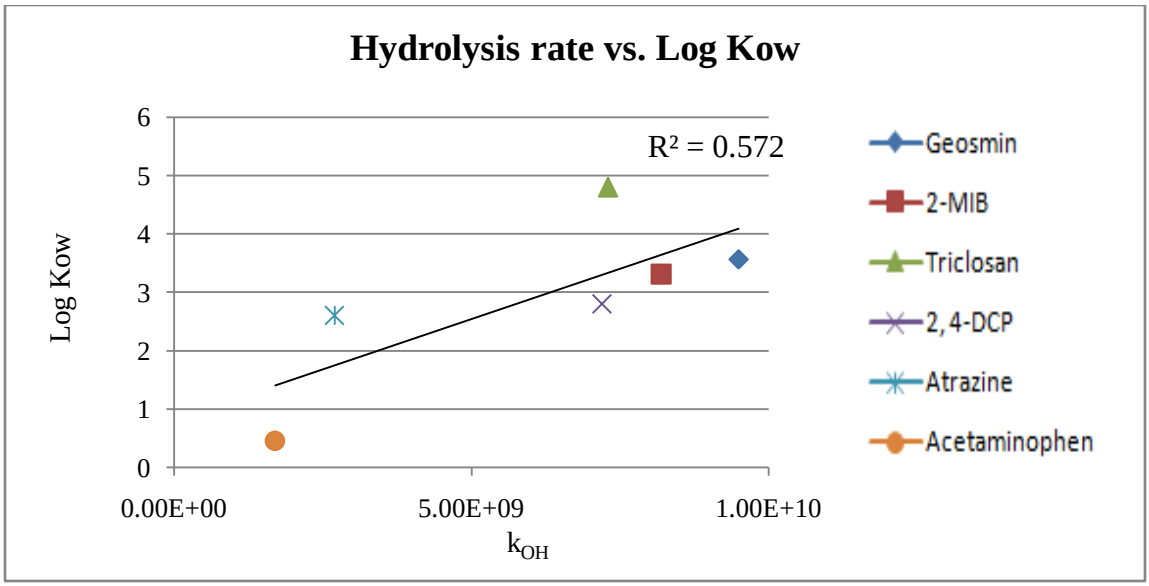


Figure 42 Log octanol-water partition coefficient vs. Hydrolysis rate constant.

In this study it was found that for most of the descriptors used displayed low correlations between physical-chemical properties and degradation rate. There are many reasons for this. One of them and likely the most important may be the data for biodegradation rate, oxidation rate and hydrolysis rate extracted from literature were not studied and calculated under same conditions. For more accuracy it may be useful to calculate data under same conditions. This will reduce or remove the experimental error which may have occurred in the respective studies. Also, when data are calculated under the same conditions the error, if any, will be same for all the data. Another reason for the correlation to not exist between the descriptors and rate constant may be the amount of data. In our study only six compounds were used. In this type of study the number of compounds should have been more for better correlations. Also, these six compounds are from heterologous groups with different structural, physical and chemical properties.

Increasing the size of our data set may have resulted in better correlations between the descriptors and rate constants.

CHAPTER V

CONCLUSION

5.1 Conclusions

In the study an attempt was made to find correlations between physical chemical properties of geosmin, 2-methylisobrneol, 2,4-dichlorophenol, acetaminophen, atrazine and triclosan with the biodegradation, oxidation and hydrolysis rate constants. In doing so, various physical chemical properties, quantum chemical properties and structural properties and also the biodegradation, oxidation and hydrolysis rate constants were found, presenting us with valuable information about the chemicals used in the study. The data itself is thus a contribution on its own.

A preliminary analysis is provided from this study that can be used for a full scale quantitative structure analysis relationship. From the study, correlations were found somewhat promising for

1. biodegradation rate constant and log octanol-air partition coefficient ($R^2 = 0.432$)
2. oxidation rate constant and E_{HOMO} ($R^2 = 0.309$)
3. hydrolysis rate constant and E_{LUMO} ($R^2 = 0.746$)
4. hydrolysis rate constant and E_{HOMO} ($R^2 = 0.505$)
5. hydrolysis rate constant and log octanol-water partition coefficient ($R^2 = 0.572$)

5.2 Recommendations for Further Research

There is variety of directions for further work. Based on the results obtained from the study, the following recommendations are addressed

- One possibility is to increase the data set by increasing the number of chemicals. In this study one six compounds were used. Additions of well studied chemicals for which data may be easily available should be included for full-scale QSARs.
- Data for activity rates (biodegradation, oxidation and hydrolysis rate constants) should be relevant, meaning, studied under same condition. Whenever possible, it is desirable to compile data for a particular measurement from references originating within the same laboratory and measurement system. Data quality and compatibility of data may be an important parameter in this type of study.
- A good model to predict chemicals fate in environment can be obtained by combining physicochemical and molecular-orbital properties when there is no significant correlation between them. Statistical analysis should be performed using variety of descriptors to better understand the correlations between molecular descriptors and fate of chemicals in environment.
- There are many methods available to build a QSAR model that can relate activity to molecular structure. Some methods are designed to work with data that are measured on a nominal or ordinal scale, meaning the results are divided into two or more classes that may bear some relation to one another. These techniques should be explored further.

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APPPENDICES

APPENDIX A MOLECULAR MODELING PRO

The Molecular Modeling Pro program uses the computational chemistry method for calculation of various physical properties of chemicals. The software is available to download at http//www.chemsw.com/13052.htm.

The Molecular Modeling Pro is an interface program developed by ChemSW for Windows. The program estimates various physical properties like mass, sizes, partition coefficients, hydrophobicity, solubility, thermodynamics, properties used for QSAR studies and many other properties of chemicals. The Molecular Modeling Pro is

- a physical property estimation program
- a 3-D chemical structure drawing program
- a chemical data base creation program (used with the companion Molecular Analysis Pro program)
- a molecular graphics modeling tool
- a reaction/mixture editor
- a computer slide show maker
- a batch structure printing program

In the study the software was used to calculate the energy of highest occupied molecular orbital (E_{HOMO}) and energy of lowest unoccupied molecular orbital (E_{LUMO}). The ouput from the program for geosmin as example is presented below

```
**********************************************************************
**********
 **   32-bit Microsoft Windows, Victor Lobanov, 1996, University of Florida   **
 **     max number of heavy atoms =  50, max number of light atoms = 100      **

**********************************************************************
**********

                          AM1 CALCULATION RESULTS


**********************************************************************
**********
 *         MOPAC  VERSION  6.00            CALC'D.
 *  VECTORS  - FINAL EIGENVECTORS TO BE PRINTED
 *   T=      - A TIME OF  3600.0 SECONDS REQUESTED
 *  DUMP=N   - RESTART FILE WRITTEN EVERY  3600.0 SECONDS
 *  1SCF     - DO 1 SCF AND THEN STOP
 *  AM1      - THE AM1 HAMILTONIAN TO BE USED

**********************************************************************
*****050BY100
 1SCF    AM1   VECTORS  T=3600
 Molecule-1
 MOPAC calculations

   ATOM   CHEMICAL  BOND LENGTH    BOND ANGLE     TWIST ANGLE
  NUMBER  SYMBOL    (ANGSTROMS)    (DEGREES)      (DEGREES)
   (I)              NAI        NBNAI     NCNBNAI     NA   NB   NC

     1     O
     2     C       1.54883  *                          1
     3     C       1.54883  *    108.65790  *             2    1
```

4	C	1.54950	*	109.56250	*	-59.25550	*	3 2 1
5	H	.98719	*	110.35230	*	179.81210	*	1 2 3
6	H	.99999	*	109.44030	*	-179.26520	*	3 2 1
7	H	1.00004	*	109.43290	*	60.74217	*	3 2 1
8	C	1.54905	*	109.41190	*	-59.76140	*	4 3 2
9	H	.99996	*	109.47920	*	-179.73960	*	4 3 2
10	H	.99994	*	109.48040	*	60.21403	*	4 3 2
11	C	1.54904	*	109.72890	*	59.65221	*	8 4 3
12	H	.99997	*	109.39990	*	-60.37520	*	8 4 3
13	H	1.00000	*	109.39790	*	179.68080	*	8 4 3
14	C	1.54577	*	109.85980	*	-60.39690	*	11 8 4
15	H	1.00004	*	109.36450	*	179.56100	*	11 8 4
16	H	1.00001	*	109.36870	*	59.65016	*	11 8 4
17	C	1.56397	*	108.84530	*	-61.81910	*	14 11 8
18	C	1.54714	*	109.79920	*	178.91590	*	14 11 8
19	C	1.55859	*	110.05240	*	-178.55780	*	2 3 4
20	C	1.54062	*	109.59960	*	59.85987	*	19 2 3
21	C	1.54984	*	109.42190	*	179.70300	*	19 2 3
22	H	1.09755	*	110.06380	*	-60.14360	*	19 2 3
23	C	1.55179	*	109.37580	*	59.49637	*	21 19 2
24	H	.99992	*	109.49340	*	-60.47570	*	21 19 2
25	H	1.00001	*	109.48760	*	179.46750	*	21 19 2
26	H	1.00004	*	109.38960	*	59.72116	*	23 21 19
27	H	.99998	*	109.39280	*	179.66230	*	23 21 19
28	H	.99997	*	109.50240	*	-60.08640	*	20 19 2
29	H	1.00011	*	109.49870	*	179.92070	*	20 19 2
30	H	.99998	*	109.50380	*	59.91640	*	20 19 2
31	H	.99994	*	109.49720	*	180.00000	*	17 14 11
32	H	1.00007	*	109.49390	*	59.99722	*	17 14 11
33	H	1.00003	*	109.49830	*	-60.00450	*	17 14 11
34	H	1.00000	*	109.37450	*	-58.35430	*	18 14 11
35	H	1.00003	*	109.37460	*	61.55955	*	18 14 11

CARTESIAN COORDINATES

NO.	ATOM	X	Y	Z
1	O	.0000	.0000	.0000
2	C	1.5488	.0000	.0000

3	C	2.0443	1.4674	.0000
4	C	1.5031	2.1978	-1.2549
5	H	-.3433	-.9256	-.0030
6	H	3.0442	1.4811	-.0121
7	H	1.7141	1.9301	.8228
8	C	2.0100	1.4768	-2.5288
9	H	1.8272	3.1438	-1.2558
10	H	.5033	2.1875	-1.2414
11	C	1.5189	.0077	-2.5286
12	H	3.0097	1.4928	-2.5440
13	H	1.6564	1.9452	-3.3384
14	C	2.0685	-.7296	-1.2862
15	H	1.8430	-.4503	-3.3564
16	H	.5192	-.0078	-2.5081
17	C	3.6309	-.7397	-1.3549
18	C	1.5549	-2.1890	-1.2731
19	C	2.0568	-.7356	1.2768
20	C	1.5230	-.0198	2.5323
21	C	1.5468	-2.1991	1.2656
22	H	3.1540	-.7335	1.3011
23	C	2.0735	-2.9181	-.0047
24	H	.5469	-2.2040	1.2612
25	H	1.8794	-2.6744	2.0801
26	H	3.0735	-2.9080	-.0013
27	H	1.7492	-3.8640	-.0093
28	H	1.8504	.9250	2.5425
29	H	1.8488	-.4937	3.3506
30	H	.5232	-.0255	2.5202
31	H	3.9971	-1.2149	-.5549
32	H	3.9705	.2008	-1.3679
33	H	3.9255	-1.2116	-2.1860
34	H	.5549	-2.1887	-1.2701
35	H	1.8862	-2.6646	-2.0880

H (AM1) M.J.S. DEWAR ET AL, J. AM. CHEM. SOC. 107 3902-3909 (1985)
C (AM1) M.J.S. DEWAR ET AL, J. AM. CHEM. SOC. 107 3902-3909 (1985)
O (AM1) M.J.S. DEWAR ET AL, J. AM. CHEM. SOC. 107 3902-3909 (1985)

RHF CALCULATION, NO. OF DOUBLY OCCUPIED LEVELS = 38

INTERATOMIC DISTANCES

0

		O 1	C 2	C 3	C 4	H 5	H 6
O	1	.000000					
C	2	1.548832	.000000				
C	3	2.516475	1.548832	.000000			
C	4	2.943524	2.531203	1.549502	.000000		
H	5	.987188	2.106409	3.380436	3.838196	.000000	
H	6	3.385370	2.104718	.999993	2.105422	4.155386	.000000
H	7	2.709311	2.104665	1.000044	2.105385	3.615214	1.633311
C	8	3.551886	2.964533	2.529032	1.549052	4.205838	2.720884
H	9	3.846955	3.396733	2.105765	.999962	4.779136	2.406681
H	10	2.565066	2.723832	2.105765	.999941	3.455642	2.909629
C	11	2.949737	2.528820	2.966626	2.533599	3.273740	3.290958
H	12	4.214111	3.291578	2.721093	2.104408	4.852621	2.532122
H	13	4.203884	3.865312	3.394687	2.104402	4.833752	3.633985
C	14	2.542701	1.567382	2.545955	2.981649	2.738951	2.731765
H	15	3.855483	3.399231	3.870904	3.397730	4.031224	4.044484
H	16	2.561323	2.711278	3.285282	2.720906	2.803894	3.850005
C	17	3.945450	2.591920	3.037198	3.628558	4.202004	2.660737
C	18	2.971557	2.532257	3.902497	4.387095	2.610110	4.156598
C	19	2.530116	1.558588	2.546270	3.914095	2.726627	2.747683
C	20	2.955101	2.532513	2.982657	4.388708	3.275922	3.322733
C	21	2.971579	2.537251	3.910558	5.068222	2.608441	4.173514
H	22	3.489818	2.192609	2.787169	4.224999	3.737555	2.577001
C	23	3.579787	2.964903	4.385635	5.297224	3.132331	4.505026
H	24	2.597567	2.729843	4.160791	5.159508	2.006319	4.630055
H	25	3.874485	3.404235	4.637806	5.916265	3.512641	4.796112
H	26	4.231219	3.283503	4.494892	5.486982	3.950332	4.389273
H	27	4.241501	3.869213	5.339616	6.193318	3.607385	5.499755
H	28	3.277798	2.722292	2.606950	4.020021	3.836249	2.874068
H	29	3.858486	3.399991	3.887244	5.345423	4.029680	4.078774
H	30	2.574018	2.721008	3.300616	4.489338	2.815568	3.877843
H	31	4.214337	2.788879	3.363933	4.284405	4.384930	2.910522
H	32	4.204329	2.788540	2.680582	3.176231	4.662706	2.082158
H	33	4.653549	3.448862	3.936252	4.284645	4.803078	3.571118
H	34	2.590705	2.718747	4.147175	4.487855	2.002013	4.609403
H	35	3.875248	3.401996	4.632313	4.948077	3.513144	4.778811

1
0

	H 7	C 8	H 9	H 10	C 11	H 12
H 7	.000000					
C 8	3.394983	.000000				
H 9	2.409599	2.105362	.000000			
H 10	2.406863	2.105312	1.633208	.000000		
C 11	3.868540	1.549042	3.398527	2.727551	.000000	
H 12	3.633831	.999969	2.404830	2.908796	2.104406	.000000
H 13	4.161617	.999995	2.408933	2.405319	2.104448	1.633230
C 14	3.412844	2.532949	3.881000	3.310763	1.545771	2.721604
H 15	4.811310	2.104020	4.162985	3.636736	1.000038	2.407781
H 16	4.034616	2.104050	3.634762	2.534545	1.000009	2.907911
C 17	3.942661	2.986396	4.283063	4.285233	2.529272	2.604629
C 18	4.624364	3.901542	5.339710	4.501135	2.530453	4.157794
C 19	2.725697	4.402173	4.638511	4.159162	3.914449	4.524582
C 20	2.600253	5.300161	4.944752	4.489213	5.061011	5.501525
C 21	4.156226	5.303222	5.914551	5.159052	4.389412	5.502999
H 22	3.065462	4.567517	4.830229	4.692825	4.229655	4.445408
C 23	4.931440	5.068598	6.194533	5.482888	3.903655	5.175022
H 24	4.318013	5.482081	6.047560	5.054712	4.494369	5.849044
H 25	4.776007	6.204206	6.706908	6.046856	5.344587	6.326610
H 26	5.092642	5.171696	6.304874	5.840215	4.160059	5.083009
H 27	5.853681	5.911029	7.118194	6.300059	4.624954	6.058802
H 28	1.996598	5.103720	4.398938	4.210302	5.164080	5.247716
H 29	3.504707	6.202882	5.869447	5.485015	5.909746	6.327680
H 30	2.850252	5.473536	5.099294	4.364317	5.146148	5.842405
H 31	4.123245	3.884617	4.919094	4.924817	3.395910	3.501875
H 32	3.588986	2.611403	3.642387	3.997996	2.719422	1.993863
H 33	4.879836	3.318727	4.923068	4.914927	2.719523	2.877581
H 34	4.763271	4.139786	5.482198	4.376619	2.708759	4.604627
H 35	5.441828	4.166649	5.867960	5.115815	2.733187	4.330628

1
0

	H 13	C 14	H 15	H 16	C 17	C 18
H 13	.000000					
C 14	3.396522	.000000				
H 15	2.402920	2.101100	.000000			

H	16	2.407662	2.101102	1.633349	.000000		
C	17	3.878451	1.563972	2.699384	3.398352	.000000	
C	18	4.622529	1.547141	2.728747	2.712179	2.533125	.000000
C	19	5.352299	2.563003	4.646869	4.149634	3.066537	2.977564
C	20	6.192314	3.922022	5.913085	5.139455	4.480144	4.380300
C	21	6.195519	2.990513	4.950630	4.483198	3.652426	2.538711
H	22	5.562705	2.805792	4.846790	4.688225	2.698457	3.361822
C	23	5.911023	2.536111	4.168593	4.141682	2.998990	1.552228
H	24	6.293158	3.313365	5.106618	4.362610	4.301076	2.727461
H	25	7.124041	3.892335	5.873994	5.478463	4.313975	3.403652
H	26	6.057989	2.721510	4.337204	4.606581	2.616213	2.107252
H	27	6.696190	3.399531	4.781712	4.756852	3.887498	2.107251
H	28	5.971929	4.176623	6.057121	5.305775	4.596861	4.933818
H	29	7.122367	4.647940	6.707099	6.027295	5.037636	4.933351
H	30	6.284195	4.168000	6.037914	5.028338	5.018404	4.487063
H	31	4.818055	2.118921	3.615724	4.167540	.999945	2.725572
H	32	3.504458	2.118974	2.984086	3.640800	1.000074	3.399285
H	33	4.054919	2.118995	2.507230	3.627079	1.000029	2.721769
H	34	4.751932	2.102417	3.005584	2.508114	3.401249	1.000003
H	35	4.781941	2.102438	2.552169	3.017287	2.699368	1.000031

0

		C 19	C 20	C 21	H 22	C 23	H 24
C	19	.000000					
C	20	1.540615	.000000				
C	21	1.549837	2.520738	.000000			
H	22	1.097551	2.164567	2.175401	.000000		
C	23	2.530974	3.890914	1.551787	2.764973	.000000	
H	24	2.106204	2.709040	.999915	2.993498	2.107846	.000000
H	25	2.106202	2.716320	1.000010	2.449285	2.107940	1.633205
H	26	2.717887	4.143051	2.106776	2.536029	1.000035	2.910902
H	27	3.396449	4.613980	2.106777	3.673020	.999983	2.411540
H	28	2.098108	.999969	3.388545	2.447660	4.615961	3.623682
H	29	2.098166	1.000111	2.710394	2.441623	4.145536	2.997480
H	30	2.098131	.999977	2.710368	2.984784	4.140710	2.516178
H	31	2.711007	4.132766	3.207277	2.094536	2.627504	4.022469
H	32	3.396094	4.609796	4.309188	2.943292	3.896757	4.941291
H	33	3.963471	5.427139	4.306558	3.603215	3.331665	4.927735
H	34	3.294517	4.483283	2.722841	3.934999	2.107002	2.531422
H	35	3.882255	5.336087	3.402737	4.101524	2.107051	3.636381

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0

		H 25	H 26	H 27	H 28	H 29	H 30
H	25	.000000					
H	26	2.410981	.000000				
H	27	2.407881	1.633327	.000000			
H	28	3.629109	4.760143	5.427389	.000000		
H	29	2.523951	4.308563	4.759983	1.632704	.000000	
H	30	3.008288	4.601203	4.757689	1.632650	1.632797	.000000
H	31	3.682150	2.006553	3.516897	4.333706	4.515274	4.789439
H	32	4.952658	3.512460	4.827314	4.506692	5.219947	5.201188
H	33	4.952369	2.894246	4.063170	5.588289	5.956583	5.927054
H	34	3.635135	2.910410	2.412951	5.090147	5.088967	4.364268
H	35	4.168146	2.413151	2.403799	5.858994	5.855918	5.482499

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		H 31	H 32	H 33	H 34	H 35
H	31	.000000				
H	32	1.632786	.000000			
H	33	1.632667	1.632841	.000000		
H	34	3.648063	4.169617	3.626840	.000000	
H	35	2.984619	3.615736	2.505873	1.633283	.000000

1SCF AM1 VECTORS T=3600
Molecule-1
MOPAC calculations

1SCF WAS SPECIFIED, SO BFGS WAS NOT USED
SCF FIELD WAS ACHIEVED

AM1 CALCULATION
VERSION 6.00

FINAL HEAT OF FORMATION = 47.72085 KCAL

TOTAL ENERGY = -2155.75281 EV
ELECTRONIC ENERGY = -14991.18584 EV
CORE-CORE REPULSION = 12835.43303 EV

IONIZATION POTENTIAL = 10.45765
NO. OF FILLED LEVELS = 38
MOLECULAR WEIGHT = 182.305

SCF CALCULATIONS = 1
COMPUTATION TIME = .140 SECONDS

ATOM NUMBER (I)	CHEMICAL SYMBOL	BOND LENGTH (ANGSTROMS) NAI		BOND ANGLE (DEGREES) NBNAI		TWIST ANGLE (DEGREES) NCNBNAI		NA	NB	NC
1	O									
2	C	1.54883	*					1		
3	C	1.54883	*	108.65790	*			2	1	
4	C	1.54950	*	109.56250	*	-59.25550	*	3	2	1
5	H	.98719	*	110.35230	*	179.81210	*	1	2	3
6	H	.99999	*	109.44030	*	-179.26520	*	3	2	1
7	H	1.00004	*	109.43290	*	60.74217	*	3	2	1
8	C	1.54905	*	109.41190	*	-59.76140	*	4	3	2
9	H	.99996	*	109.47920	*	-179.73960	*	4	3	2
10	H	.99994	*	109.48040	*	60.21403	*	4	3	2
11	C	1.54904	*	109.72890	*	59.65221	*	8	4	3
12	H	.99997	*	109.39990	*	-60.37520	*	8	4	3
13	H	1.00000	*	109.39790	*	179.68080	*	8	4	3
14	C	1.54577	*	109.85980	*	-60.39690	*	11	8	4
15	H	1.00004	*	109.36450	*	179.56100	*	11	8	4
16	H	1.00001	*	109.36870	*	59.65016	*	11	8	4

17	C	1.56397	*	108.84530	*	-61.81910	*	14	11	8
18	C	1.54714	*	109.79920	*	178.91590	*	14	11	8
19	C	1.55859	*	110.05240	*	-178.55780	*	2	3	4
20	C	1.54062	*	109.59960	*	59.85987	*	19	2	3
21	C	1.54984	*	109.42190	*	179.70300	*	19	2	3
22	H	1.09755	*	110.06380	*	-60.14360	*	19	2	3
23	C	1.55179	*	109.37580	*	59.49637	*	21	19	2
24	H	.99992	*	109.49340	*	-60.47570	*	21	19	2
25	H	1.00001	*	109.48760	*	179.46750	*	21	19	2
26	H	1.00004	*	109.38960	*	59.72116	*	23	21	19
27	H	.99998	*	109.39280	*	179.66230	*	23	21	19
28	H	.99997	*	109.50240	*	-60.08640	*	20	19	2
29	H	1.00011	*	109.49870	*	179.92070	*	20	19	2
30	H	.99998	*	109.50380	*	59.91640	*	20	19	2
31	H	.99994	*	109.49720	*	180.00000	*	17	14	11
32	H	1.00007	*	109.49390	*	59.99722	*	17	14	11
33	H	1.00003	*	109.49830	*	-60.00450	*	17	14	11
34	H	1.00000	*	109.37450	*	-58.35430	*	18	14	11
35	H	1.00003	*	109.37460	*	61.55955	*	18	14	11

INTERATOMIC DISTANCES

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		O 1	C 2	C 3	C 4	H 5	H 6
O	1	.000000					
C	2	1.548832	.000000				
C	3	2.516475	1.548832	.000000			
C	4	2.943524	2.531203	1.549502	.000000		
H	5	.987188	2.106409	3.380436	3.838196	.000000	
H	6	3.385370	2.104718	.999993	2.105422	4.155386	.000000
H	7	2.709311	2.104665	1.000044	2.105385	3.615214	1.633311
C	8	3.551886	2.964533	2.529032	1.549052	4.205838	2.720884
H	9	3.846955	3.396733	2.105765	.999962	4.779136	2.406681
H	10	2.565066	2.723832	2.105765	.999941	3.455642	2.909629
C	11	2.949737	2.528820	2.966626	2.533599	3.273740	3.290958
H	12	4.214111	3.291578	2.721093	2.104408	4.852621	2.532122
H	13	4.203884	3.865312	3.394687	2.104402	4.833752	3.633985
C	14	2.542701	1.567382	2.545955	2.981649	2.738951	2.731765
H	15	3.855483	3.399231	3.870904	3.397730	4.031224	4.044484

H	16	2.561323	2.711278	3.285282	2.720906	2.803894	3.850005
C	17	3.945450	2.591920	3.037198	3.628558	4.202004	2.660737
C	18	2.971557	2.532257	3.902497	4.387095	2.610110	4.156598
C	19	2.530116	1.558588	2.546270	3.914095	2.726627	2.747683
C	20	2.955101	2.532513	2.982657	4.388708	3.275922	3.322733
C	21	2.971579	2.537251	3.910558	5.068222	2.608441	4.173514
H	22	3.489818	2.192609	2.787169	4.224999	3.737555	2.577001
C	23	3.579787	2.964903	4.385635	5.297224	3.132331	4.505026
H	24	2.597567	2.729843	4.160791	5.159508	2.006319	4.630055
H	25	3.874485	3.404235	4.637806	5.916265	3.512641	4.796112
H	26	4.231219	3.283503	4.494892	5.486982	3.950332	4.389273
H	27	4.241501	3.869213	5.339616	6.193318	3.607385	5.499755
H	28	3.277798	2.722292	2.606950	4.020021	3.836249	2.874068
H	29	3.858486	3.399991	3.887244	5.345423	4.029680	4.078774
H	30	2.574018	2.721008	3.300616	4.489338	2.815568	3.877843
H	31	4.214337	2.788879	3.363933	4.284405	4.384930	2.910522
H	32	4.204329	2.788540	2.680582	3.176231	4.662706	2.082158
H	33	4.653549	3.448862	3.936252	4.284645	4.803078	3.571118
H	34	2.590705	2.718747	4.147175	4.487855	2.002013	4.609403
H	35	3.875248	3.401996	4.632313	4.948077	3.513144	4.778811

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	H 7	C 8	H 9	H 10	C 11	H 12
H	7	.000000				
C	8	3.394983	.000000			
H	9	2.409599	2.105362	.000000		
H	10	2.406863	2.105312	1.633208	.000000	
C	11	3.868540	1.549042	3.398527	2.727551	.000000
H	12	3.633831	.999969	2.404830	2.908796	2.104406	.000000
H	13	4.161617	.999995	2.408933	2.405319	2.104448	1.633230
C	14	3.412844	2.532949	3.881000	3.310763	1.545771	2.721604
H	15	4.811310	2.104020	4.162985	3.636736	1.000038	2.407781
H	16	4.034616	2.104050	3.634762	2.534545	1.000009	2.907911
C	17	3.942661	2.986396	4.283063	4.285233	2.529272	2.604629
C	18	4.624364	3.901542	5.339710	4.501135	2.530453	4.157794
C	19	2.725697	4.402173	4.638511	4.159162	3.914449	4.524582
C	20	2.600253	5.300161	4.944752	4.489213	5.061011	5.501525
C	21	4.156226	5.303222	5.914551	5.159052	4.389412	5.502999
H	22	3.065462	4.567517	4.830229	4.692825	4.229655	4.445408

C	23	4.931440	5.068598	6.194533	5.482888	3.903655	5.175022
H	24	4.318013	5.482081	6.047560	5.054712	4.494369	5.849044
H	25	4.776007	6.204206	6.706908	6.046856	5.344587	6.326610
H	26	5.092642	5.171696	6.304874	5.840215	4.160059	5.083009
H	27	5.853681	5.911029	7.118194	6.300059	4.624954	6.058802
H	28	1.996598	5.103720	4.398938	4.210302	5.164080	5.247716
H	29	3.504707	6.202882	5.869447	5.485015	5.909746	6.327680
H	30	2.850252	5.473536	5.099294	4.364317	5.146148	5.842405
H	31	4.123245	3.884617	4.919094	4.924817	3.395910	3.501875
H	32	3.588986	2.611403	3.642387	3.997996	2.719422	1.993863
H	33	4.879836	3.318727	4.923068	4.914927	2.719523	2.877581
H	34	4.763271	4.139786	5.482198	4.376619	2.708759	4.604627
H	35	5.441828	4.166649	5.867960	5.115815	2.733187	4.330628

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		H 13	C 14	H 15	H 16	C 17	C 18
H	13	.000000					
C	14	3.396522	.000000				
H	15	2.402920	2.101100	.000000			
H	16	2.407662	2.101102	1.633349	.000000		
C	17	3.878451	1.563972	2.699384	3.398352	.000000	
C	18	4.622529	1.547141	2.728747	2.712179	2.533125	.000000
C	19	5.352299	2.563003	4.646869	4.149634	3.066537	2.977564
C	20	6.192314	3.922022	5.913085	5.139455	4.480144	4.380300
C	21	6.195519	2.990513	4.950630	4.483198	3.652426	2.538711
H	22	5.562705	2.805792	4.846790	4.688225	2.698457	3.361822
C	23	5.911023	2.536111	4.168593	4.141682	2.998990	1.552228
H	24	6.293158	3.313365	5.106618	4.362610	4.301076	2.727461
H	25	7.124041	3.892335	5.873994	5.478463	4.313975	3.403652
H	26	6.057989	2.721510	4.337204	4.606581	2.616213	2.107252
H	27	6.696190	3.399531	4.781712	4.756852	3.887498	2.107251
H	28	5.971929	4.176623	6.057121	5.305775	4.596861	4.933818
H	29	7.122367	4.647940	6.707099	6.027295	5.037636	4.933351
H	30	6.284195	4.168000	6.037914	5.028338	5.018404	4.487063
H	31	4.818055	2.118921	3.615724	4.167540	.999945	2.725572
H	32	3.504458	2.118974	2.984086	3.640800	1.000074	3.399285
H	33	4.054919	2.118995	2.507230	3.627079	1.000029	2.721769
H	34	4.751932	2.102417	3.005584	2.508114	3.401249	1.000003
H	35	4.781941	2.102438	2.552169	3.017287	2.699368	1.000031

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		C 19	C 20	C 21	H 22	C 23	H 24
C	19	.000000					
C	20	1.540615	.000000				
C	21	1.549837	2.520738	.000000			
H	22	1.097551	2.164567	2.175401	.000000		
C	23	2.530974	3.890914	1.551787	2.764973	.000000	
H	24	2.106204	2.709040	.999915	2.993498	2.107846	.000000
H	25	2.106202	2.716320	1.000010	2.449285	2.107940	1.633205
H	26	2.717887	4.143051	2.106776	2.536029	1.000035	2.910902
H	27	3.396449	4.613980	2.106777	3.673020	.999983	2.411540
H	28	2.098108	.999969	3.388545	2.447660	4.615961	3.623682
H	29	2.098166	1.000111	2.710394	2.441623	4.145536	2.997480
H	30	2.098131	.999977	2.710368	2.984784	4.140710	2.516178
H	31	2.711007	4.132766	3.207277	2.094536	2.627504	4.022469
H	32	3.396094	4.609796	4.309188	2.943292	3.896757	4.941291
H	33	3.963471	5.427139	4.306558	3.603215	3.331665	4.927735
H	34	3.294517	4.483283	2.722841	3.934999	2.107002	2.531422
H	35	3.882255	5.336087	3.402737	4.101524	2.107051	3.636381

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0

		H 25	H 26	H 27	H 28	H 29	H 30
H	25	.000000					
H	26	2.410981	.000000				
H	27	2.407881	1.633327	.000000			
H	28	3.629109	4.760143	5.427389	.000000		
H	29	2.523951	4.308563	4.759983	1.632704	.000000	
H	30	3.008288	4.601203	4.757689	1.632650	1.632797	.000000
H	31	3.682150	2.006553	3.516897	4.333706	4.515274	4.789439
H	32	4.952658	3.512460	4.827314	4.506692	5.219947	5.201188
H	33	4.952369	2.894246	4.063170	5.588289	5.956583	5.927054
H	34	3.635135	2.910410	2.412951	5.090147	5.088967	4.364268
H	35	4.168146	2.413151	2.403799	5.858994	5.855918	5.482499

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		H 31	H 32	H 33	H 34	H 35
H	31	.000000				
H	32	1.632786	.000000			

H	33	1.632667	1.632841	.000000	
H	34	3.648063	4.169617	3.626840	.000000
H	35	2.984619	3.615736	2.505873	1.633283	.000000

EIGENVECTORS

ROOT NO.	1	2	3	4	5	6
	-41.72852	-37.47058	-35.83598	-34.41517	-32.28531	-31.21230
S O 1	.20043	-.07781	-.42487	.72639	-.12119	.10961
PX O 1	.06428	-.00280	-.06097	.03103	.02449	-.03870
PY O 1	-.03024	.03470	.03540	-.10308	.01727	-.04046
PZ O 1	-.00425	-.01851	-.01792	-.01452	.00607	.00301
S C 2	.35148	-.01364	-.22773	.07029	.15787	-.19476
PX C 2	.01759	.01860	.07395	-.16238	.07657	-.07025
PY C 2	-.02290	.09682	-.07164	-.04223	-.02992	-.10313
PZ C 2	-.02390	-.09014	-.09651	-.07136	.00397	.02139
S C 3	.23736	.20677	-.25363	-.15790	-.03873	-.42991
PX C 3	-.01825	-.01431	.03430	-.01302	.02607	.00793
PY C 3	-.05027	.02942	.01994	-.02619	-.08988	.00566
PZ C 3	-.03120	-.07989	-.00808	.01157	.06666	.00444
S C 4	.19120	.33512	-.15437	-.17762	-.30453	-.14377
PX C 4	.02054	.03238	-.00906	-.02291	-.01179	-.01680
PY C 4	-.05081	-.05404	.01546	.00833	.00150	-.00333
PZ C 4	.00443	-.02698	-.04684	-.00364	.03846	-.15983
S H 5	.08588	-.04938	-.12017	.23503	-.04924	.05309
S H 6	.09907	.08281	-.08749	-.07339	.00387	-.17861
S H 7	.08500	.06081	-.11750	-.06993	-.00849	-.17317

S C 8	.20091	.36481	.00771	-.11552	-.23371	.32615
PX C 8	-.01364	-.02684	.00644	.00464	.03104	-.02422
PY C 8	-.03495	-.02191	-.04950	-.03034	-.06428	-.09289
PZ C 8	.04110	.05436	-.03139	-.02806	-.03615	-.07176
S H 9	.06294	.12235	-.05981	-.07447	-.12986	-.06504
S H 10	.07447	.12573	-.06317	-.05840	-.12190	-.05077
S C 11	.24992	.27852	.16705	.03843	.03234	.40136
PX C 11	.02908	.02857	.02829	-.00640	.03240	.00965
PY C 11	.00046	.06914	-.04919	-.04981	-.08703	.06269
PZ C 11	.06081	.01959	.01825	.02253	.04210	-.04624
S H 12	.08398	.14334	.00982	-.04674	-.07433	.12064
S H 13	.06537	.13288	.00323	-.04533	-.10455	.14942
S C 14	.37282	.08323	.25727	.12240	.26327	-.02608
PX C 14	-.01134	.00590	.03529	-.03706	.09304	-.05195
PY C 14	.00905	.09590	-.08735	-.02597	.03498	.04334
PZ C 14	.02442	-.07201	-.06915	-.00695	.00362	-.12819
S H 15	.08986	.09913	.08081	.01807	.02301	.17490
S H 16	.09751	.10299	.05411	.02603	-.00418	.16205
S C 17	.21632	.06557	.22653	.03490	.37708	-.12067
PX C 17	-.06864	-.01667	-.04949	-.01892	-.03991	-.00098
PY C 17	.00409	.03109	-.02280	-.01040	.00865	.00940
1						
PZ C 17	.01093	-.02019	-.01169	-.00819	.00352	-.03530
S C 18	.26565	-.14923	.33419	.11889	-.10734	-.11409
PX C 18	.02718	-.00936	.04321	-.00645	.02155	-.02501
PY C 18	.05210	.03927	.01571	.03437	.10695	.02219
PZ C 18	.03619	-.06916	.01291	-.01510	-.07659	-.03367
S C 19	.26751	-.28046	-.22796	-.24264	.14526	.12431

PX C 19	-.03027	.03771	.04641	-.00031	.00402	-.03431
PY C 19	-.00190	.05962	-.07152	.00503	.11143	-.03709
PZ C 19	-.04677	-.01945	-.03253	-.06940	.01485	.11572
S C 20	.13621	-.18680	-.25820	-.26203	.23003	.26728
PX C 20	.01016	-.01126	-.01078	-.02339	.01488	.00348
PY C 20	-.01820	.03807	.01076	.02474	.00428	-.03521
PZ C 20	-.04421	.03781	.04879	.03049	-.02375	.00034
S C 21	.22193	-.34801	.00408	-.17881	-.25345	.11540
PX C 21	.01845	-.02521	.01227	-.02589	-.00838	-.00689
PY C 21	.03554	-.02644	-.07285	-.03450	.09131	.04411
PZ C 21	-.04291	.03813	-.05854	-.02399	.06672	.05267
S H 22	.09709	-.09082	-.06316	-.09416	.06495	.02626
S C 23	.22172	-.29321	.24278	-.03777	-.36813	-.10378
PX C 23	-.01849	.02761	-.01067	-.00287	.03936	-.00544
PY C 23	.05676	-.04430	.02454	-.00308	.00373	-.00274
PZ C 23	-.00743	-.03302	-.05991	-.05545	-.03538	.05174
S H 24	.09072	-.13774	-.00949	-.05368	-.10427	.05506
S H 25	.07444	-.13103	-.00394	-.08234	-.10161	.06007
S H 26	.09134	-.11089	.10116	-.01811	-.12587	-.04974
S H 27	.07285	-.10806	.09289	-.01414	-.16322	-.04165
S H 28	.05593	-.06039	-.11103	-.10554	.10151	.08629
S H 29	.04796	-.07596	-.09379	-.10833	.08755	.12277
S H 30	.05654	-.07548	-.10719	-.09340	.08695	.11140
S H 31	.09240	.00003	.08946	.00595	.14633	-.06936
S H 32	.09142	.05029	.07291	.00129	.15132	-.04792
S H 33	.07981	.02693	.10078	.01883	.14954	-.03667

S H 34	.10605	-.06001	.11516	.06251	-.05861	-.03102
S H 35	.09446	-.04518	.14077	.04742	-.03346	-.04246

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ROOT NO.	7	8	9	10	11	12
	-28.88886	-27.84454	-24.83834	-24.11586	-22.14946	-21.34627
S O 1	-.14298	.16456	.07467	-.01981	.05196	.04729
PX O 1	.04596	-.08921	-.03989	.08155	-.12485	-.05447
PY O 1	.02157	-.01983	.03994	.03341	-.03722	.00770
PZ O 1	-.01035	.01145	-.00411	.02495	.04530	.01859
S C 2	.11584	-.31549	-.13383	.25242	-.20292	-.09627
PX C 2	.00535	-.06156	-.02207	.04270	.03888	.01415
PY C 2	.01984	.02838	.20424	.02014	.09032	-.05071
PZ C 2	-.01920	.02019	-.03451	.09946	.19104	.17386
S C 3	.09389	-.06115	.31686	-.02769	.25866	-.08783
PX C 3	-.02071	-.00154	.02955	.03020	.10917	-.04903
PY C 3	-.02771	.12101	.01855	-.16774	.05865	.08372
PZ C 3	.03439	-.03429	.07917	.08286	.13148	-.01154
S C 4	-.05996	.22300	-.21080	-.27355	-.21175	.20381
PX C 4	-.01296	.00500	.01835	.04814	.09205	-.10666
PY C 4	-.01241	.04888	-.06167	-.07653	-.04055	.10025
PZ C 4	.04752	-.03007	.15819	-.11937	.04769	.05414
S H 5	-.04352	.05719	-.00528	-.05189	.06694	.00048
S H 6	.01626	-.02123	.15355	.00835	.18604	-.06940
S H 7	.05730	-.00016	.17830	-.02204	.16936	-.01641

S	C	8	-.11134	.07173	-.18023	.32566	.12963	-.23066
PX	C	8	-.02800	.01147	-.00508	.05865	.06951	-.12559
PY	C	8	-.03805	.10634	-.17492	-.00688	-.04001	-.05335
PZ	C	8	-.00617	.03475	-.03625	-.11299	-.11654	.04583
S	H	9	-.03352	.12060	-.12202	-.15292	-.10130	.13051
S	H	10	-.01697	.09024	-.09713	-.14710	-.14906	.15827
S	C	11	.13659	-.22000	.31664	-.08995	.02885	.24298
PX	C	11	-.04870	.01782	-.01316	.03690	.01381	-.10161
PY	C	11	-.07031	.02009	-.04648	.17159	.04238	-.07632
PZ	C	11	.02589	-.02494	-.05211	-.06565	-.15042	-.10584
S	H	12	-.07482	.04302	-.07898	.17884	.10668	-.18534
S	H	13	-.04847	.03983	-.10748	.18174	.08879	-.11623
S	C	14	.11171	-.11564	-.09930	-.17299	-.27586	-.16424
PX	C	14	-.20835	.10689	.02473	.04477	.03807	.01292
PY	C	14	-.07212	-.13652	.11187	.06015	-.14046	-.01758
PZ	C	14	-.01838	-.04298	-.15455	.13527	-.10637	-.10093
S	H	15	.05478	-.08168	.17149	-.04720	.08230	.16699
S	H	16	.08533	-.10038	.14160	-.06585	.00194	.17178
S	C	17	-.48085	.24196	.04188	-.00339	.05938	.03459
PX	C	17	-.06589	.05186	.03241	.04692	.10522	.06965
PY	C	17	-.01669	-.03270	.02415	.01729	-.00664	-.05122
1								
PZ	C	17	-.00487	-.01514	-.03657	.04031	-.03546	.00371
S	C	18	.38244	.23101	-.19556	-.06047	.27429	-.05858
PX	C	18	-.04183	.02742	.02337	.04613	-.08222	.05120
PY	C	18	.02241	-.08147	-.08146	-.13601	-.08859	-.07816
PZ	C	18	-.04429	-.01160	.03112	.10972	-.12324	.00245
S	C	19	-.02397	-.14064	-.27183	.08294	.17629	.36595
PX	C	19	-.01635	.00222	-.00092	.04058	.03216	.12747

PY C 19	.12518	.07935	.02609	.16390	-.04305	.03881
PZ C 19	.02230	.16867	.09577	-.11225	.03390	-.01164
S C 20	.20037	.40546	.15140	-.01954	-.15380	-.12689
PX C 20	-.00084	-.01167	-.02645	.02034	.04562	.09801
PY C 20	.03392	.03533	.06046	.04443	-.04826	-.05665
PZ C 20	.00660	.06679	.07884	-.04567	-.09582	-.14043
S C 21	-.29157	-.23971	.04444	-.30509	.07783	-.21575
PX C 21	-.01772	-.00548	.00149	.07140	-.03336	.14924
PY C 21	.02232	-.03404	-.16688	-.01648	.10600	.12708
PZ C 21	-.01713	-.00709	-.02170	-.12808	.08001	-.06029
S H 22	-.02900	-.04659	-.10465	.05982	.09401	.23387
S C 23	-.03637	.10465	.26252	.29420	-.22302	.12953
PX C 23	-.02845	.01354	.02671	.06821	-.07551	.11474
PY C 23	.00456	-.03014	-.10450	-.07642	.07119	-.04368
PZ C 23	-.15474	-.13143	.07659	-.08411	-.08182	-.06244
S H 24	-.11288	-.09469	.01855	-.17824	.05836	-.19431
S H 25	-.13853	-.09586	.05529	-.17638	.03584	-.13694
S H 26	-.04306	.05740	.12824	.17019	-.14296	.13688
S H 27	-.01213	.05767	.16557	.15879	-.12676	.06220
S H 28	.10486	.18724	.10533	.01972	-.07628	-.07483
S H 29	.07768	.18989	.08211	-.04077	-.09389	-.09503
S H 30	.08270	.17722	.08033	-.02230	-.09323	-.11859
S H 31	-.21801	.11350	.00232	.03483	.03263	.06903
S H 32	-.22591	.09699	.04020	.02707	.05900	-.01365
S H 33	-.20528	.12713	.03597	-.01758	.06916	.04394

S H 34	.18308	.08336	-.09685	-.05866	.17609	-.05905
S H 35	.16645	.12960	-.07068	-.03287	.19493	.00814

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ROOT NO.	13	14	15	16	17	18
	-19.44764	-17.50267	-16.89143	-16.48386	-15.70798	-15.44644
S O 1	-.08529	-.15979	.04303	-.01662	-.01312	.02808
PX O 1	.35021	-.23743	-.05900	.04287	.26083	.13733
PY O 1	.15626	-.42915	.06747	-.02252	.05251	.09706
PZ O 1	.03154	-.00119	-.15559	.11394	-.05312	-.06170
S C 2	.26778	.03491	.00110	.01835	-.04356	.01930
PX C 2	-.23020	.20200	.06965	-.03602	-.24292	-.08500
PY C 2	.09402	-.18441	.13957	-.00439	-.14969	-.06600
PZ C 2	.10992	.01368	-.22428	.13613	-.10232	-.00736
S C 3	-.09726	-.01923	-.02408	-.06540	.03594	-.05817
PX C 3	-.19932	.13656	.03056	.01486	.10274	.05612
PY C 3	-.11296	.01555	-.16611	.00199	.20144	.07359
PZ C 3	.01590	-.02528	-.22274	-.08859	-.16243	.14192
S C 4	.05252	.03710	.00740	.05956	-.00970	-.01062
PX C 4	-.14606	.02145	.01077	.13280	.25585	.08993
PY C 4	-.00384	.04762	-.21716	.06422	-.01078	.28246
PZ C 4	-.01492	-.02031	-.03486	.03487	.13371	-.02256
S H 5	-.17278	.34694	-.02214	.00450	-.11015	-.10245
S H 6	-.17648	.08813	.02263	-.01626	.10626	.02283
S H 7	-.02692	-.04976	-.20849	-.08961	-.04598	.08000
S C 8	-.05300	-.05514	-.01416	-.04646	-.01492	-.02559

PX C 8	-.11461	-.06660	-.03726	.25778	.19659	.15732
PY C 8	-.02328	-.02233	-.08539	-.05427	-.06495	.16149
PZ C 8	-.02467	.02915	.20288	.15367	.08965	-.11923
S H 9	-.00723	.05413	-.14038	.10602	.04991	.22062
S H 10	.12228	-.00405	.00186	-.06972	-.18599	-.07170
S C 11	.07651	.06920	-.00444	.00729	.04149	-.01480
PX C 11	-.12309	-.12633	-.06806	.28751	-.02503	-.01330
PY C 11	.04447	.04720	.11350	-.13437	-.01232	-.20088
PZ C 11	-.11289	-.04301	.18549	.08337	-.00755	-.03339
S H 12	-.09678	-.06678	-.02729	.17099	.14429	.11554
S H 13	.00663	-.03485	-.14332	-.19940	-.13841	.07386
S C 14	-.30075	-.09827	-.09177	.03773	-.07859	.02254
PX C 14	-.06707	-.06466	-.09246	.08579	-.16670	-.15526
PY C 14	.01560	.10269	.24772	.15986	-.00720	-.01645
PZ C 14	.01737	.15336	.03433	-.23068	.05089	-.02826
S H 15	.06324	.01160	-.16402	.06926	.02205	.07795
S H 16	.11724	.12167	.05445	-.20199	.03762	.00699
S C 17	.15128	.04574	.01921	-.02254	-.00098	.01071
PX C 17	.22439	.11693	.12297	-.10442	.17070	.10949
PY C 17	-.02028	.09375	.17013	.18318	.05712	.08958
1						
PZ C 17	-.04638	.07348	.05246	-.22675	.02057	-.03026
S C 18	.09753	-.03352	.06711	-.03763	.00846	-.01675
PX C 18	-.12206	-.20688	-.20721	-.03481	-.04271	-.26081
PY C 18	-.13875	-.03768	-.17731	-.14863	.05414	.15312
PZ C 18	-.03632	.17334	-.06523	-.08140	.18254	.01048
S C 19	-.10753	-.03825	.04901	.11032	.02577	-.01169
PX C 19	-.19276	-.07667	.22342	-.16127	-.10369	.22833
PY C 19	.06486	.08109	-.04726	.11948	-.25082	.11194

PZ C 19	-.06798	-.15524	.16745	.02934	.01563	-.03037
S C 20	.00607	.02989	.00361	-.02214	.02200	-.00152
PX C 20	-.08971	-.07292	.15694	-.04528	-.10063	.21895
PY C 20	.02670	.07388	-.11411	-.06574	-.15403	.19527
PZ C 20	-.02142	.01666	.07156	-.18301	.10176	.03867
S C 21	.07127	-.04274	-.01404	-.04526	-.02827	.00455
PX C 21	-.14608	-.18498	.09529	-.15467	.11442	.11346
PY C 21	-.02836	.00739	-.04729	.03520	.24804	-.23419
PZ C 21	.01169	-.17989	.13635	-.00195	-.14820	-.06059
S H 22	-.16955	-.06931	.18101	-.07632	-.05699	.16011
S C 23	-.06411	.02476	-.02643	.05213	.04340	.00315
PX C 23	-.12354	-.19069	-.06803	-.12622	.07069	-.14820
PY C 23	-.01697	.00735	-.12010	-.22950	.21224	-.06437
PZ C 23	-.03456	-.00990	-.02568	-.05234	-.04646	.22206
S H 24	.12641	.13086	-.07783	.09185	-.10357	-.08949
S H 25	.01705	-.16996	.11391	-.07661	-.16332	.07911
S H 26	-.10868	-.12022	-.06146	-.08506	.07685	-.11088
S H 27	.00565	.05069	.08409	.21665	-.14662	.08483
S H 28	-.00199	.04324	-.05160	-.07597	-.12784	.20093
S H 29	-.03475	-.02097	.12213	-.11047	.10167	.00872
S H 30	.06415	.06635	-.11445	.02754	.08174	-.16975
S H 31	.09166	.05220	.01692	-.24873	.04480	-.01474
S H 32	.09392	.11132	.15925	.10420	.10163	.10287
S H 33	.14864	-.03115	-.05639	.04496	.00076	.01542
S H 34	.12438	.15206	.18098	.00306	.03255	.18436

S H 35	.08683	-.15137	.07790	.07368	-.13704	-.13570

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ROOT NO.	19	20	21	22	23	24
	-15.05341	-14.71400	-14.45132	-14.34951	-13.99294	-13.84561
S O 1	.09301	-.14485	.12547	-.04800	.03382	.03556
PX O 1	-.06488	.10959	.01470	.06829	-.08068	-.12673
PY O 1	.23351	-.28650	.31374	-.10160	.08382	.06683
PZ O 1	-.00802	-.06429	.00888	-.11710	.06444	.00667
S C 2	-.15195	-.06844	-.12801	.04286	-.06351	.05761
PX C 2	-.00204	-.18460	-.02679	-.04494	.03755	.13294
PY C 2	.04915	-.03607	-.02978	-.05006	-.04295	.10827
PZ C 2	-.00710	-.02359	-.00038	-.16391	.02754	.03195
S C 3	.01324	.06112	.01079	.03412	-.02701	.03684
PX C 3	-.19335	-.16602	.27119	-.10757	-.02485	.13268
PY C 3	.08696	.15728	.03548	.09905	.06225	-.21402
PZ C 3	.06162	.13085	.06722	.09206	.18364	-.00501
S C 4	-.01006	-.05264	-.04097	-.04054	-.02917	-.00560
PX C 4	-.20651	-.06413	.10798	-.15695	-.18205	-.08139
PY C 4	-.14563	-.15742	.05919	.18379	.08966	.01789
PZ C 4	.09299	.00872	-.17621	.18089	-.01060	-.13492
S H 5	-.12484	.17120	-.21739	.05241	-.03874	-.00940
S H 6	-.13851	-.10851	.22163	-.06282	-.01716	.11927
S H 7	.13498	.21567	-.01256	.12087	.14174	-.11632
S C 8	.02947	.07928	.00856	-.02687	-.00728	-.02556
PX C 8	-.03922	-.05381	-.19554	.00367	-.03137	-.14475

PY	C	8	-.18109	.03257	.18589	-.00935	-.02493	.18451
PZ	C	8	-.00498	.01187	.00031	-.34905	-.09205	-.08490
S	H	9	-.16508	-.16384	.05034	.07608	.00371	-.01139
S	H	10	.15482	.01882	-.09657	.09658	.12746	.06082
S	C	11	-.00369	-.05761	-.00166	-.02577	-.00781	-.04375
PX	C	11	.14868	-.07853	-.26249	.08726	.00143	-.01885
PY	C	11	.14483	.03678	-.01942	-.00825	.03344	-.12305
PZ	C	11	.05983	.29543	.15482	-.16188	.10962	-.03867
S	H	12	-.01522	-.00278	-.14508	-.00705	-.00802	-.11869
S	H	13	-.03544	.06353	.13091	.20802	.05677	.15684
S	C	14	.06381	.07079	.11226	.06170	.03677	-.01965
PX	C	14	.11244	-.21122	-.00593	.07159	-.00749	-.00902
PY	C	14	.01526	-.02690	-.03726	.07782	.11329	-.00885
PZ	C	14	-.03251	-.14228	-.01910	.14338	-.02409	-.07524
S	H	15	-.05931	-.25593	-.17050	.11695	-.09719	.05085
S	H	16	-.11015	.04062	.20248	-.07966	.00064	-.00735
S	C	17	.01539	.02659	.02273	.01495	.00602	.00216
PX	C	17	-.12134	.12698	-.04821	-.08209	-.00428	-.00134
PY	C	17	.07249	-.13127	.00634	.09423	.39826	.02735
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PZ	C	17	-.05466	-.22672	.10219	.08281	.14094	-.44804
S	C	18	.02001	-.05422	-.03032	-.02311	.02758	-.00492
PX	C	18	-.07560	-.11843	.03833	-.02793	-.14413	-.07535
PY	C	18	.01898	.17206	.05169	-.08140	-.01201	.04071
PZ	C	18	.29936	-.02115	.08301	.06679	-.08745	.02078
S	C	19	.05767	.07301	.06648	.01223	.00783	.00155
PX	C	19	.08035	-.08125	-.10248	-.01065	-.09700	-.01285
PY	C	19	-.04257	.00784	.06685	-.09991	-.09070	-.11095
PZ	C	19	.02509	.16875	.14724	.14547	-.05205	-.08485

S C 20	-.00132	-.01591	-.00248	-.00969	-.00386	.00743
PX C 20	.10055	.04817	-.03625	.07882	-.33307	-.12428
PY C 20	.08259	-.06944	-.13243	-.35758	.06835	-.18718
PZ C 20	-.02065	-.17305	-.18395	.14293	-.13288	.18358
S C 21	.01241	-.05706	-.03374	-.06266	.00823	.00581
PX C 21	-.07469	.04470	-.21784	-.06599	.23823	.18603
PY C 21	.07636	.04170	.06082	.10378	.04081	.04234
PZ C 21	-.29809	.04063	-.00135	.15207	.05668	-.14749
S H 22	.07765	-.03109	-.03472	-.00040	-.06939	-.03635
S C 23	.04870	.03439	.02888	.00368	-.00337	.04126
PX C 23	-.29391	.08287	-.15076	-.07749	.14247	-.04747
PY C 23	.21592	-.15655	-.15820	-.20429	.00962	.09252
PZ C 23	-.01974	.06955	-.09593	-.16571	.08224	.11975
S H 24	.05571	-.05348	.14034	.01969	-.18731	-.14975
S H 25	-.23159	-.01128	-.10486	.01357	.08816	-.05633
S H 26	-.20334	.08079	-.10419	-.06446	.10246	-.03567
S H 27	-.05732	.11546	.17873	.18145	-.04842	-.03670
S H 28	.09327	-.03654	-.11012	-.24950	-.02759	-.17940
S H 29	-.02504	-.08385	-.08466	.25064	-.20885	.16966
S H 30	-.07687	-.04458	.03192	-.06950	.26668	.09938
S H 31	-.09361	-.04487	.04796	-.00773	-.05640	-.31218
S H 32	.02105	-.05767	.00321	.04560	.30365	.02430
S H 33	-.01773	.23550	-.07733	-.09973	-.25391	.30303
S H 34	.05963	.07893	-.05548	.01484	.12605	.05428

S H 35	-.20842	-.11253	-.08686	-.03323	.02910	-.04515

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ROOT NO.	25	26	27	28	29	30
	-13.53672	-13.08802	-12.89826	-12.85865	-12.59547	-12.46690
S O 1	-.04414	.00612	-.03028	.05310	-.01691	-.01433
PX O 1	.15638	.15265	.16446	-.19627	.09602	-.02317
PY O 1	-.12328	-.01621	-.09558	.12750	-.03821	-.05707
PZ O 1	-.07877	.08410	.00180	-.38097	-.25119	.19068
S C 2	.01590	-.00338	-.01158	.02983	-.05299	.00572
PX C 2	-.11193	-.08800	-.11890	.15746	-.09122	.00712
PY C 2	-.11593	-.25392	-.07657	-.00496	-.06193	-.05560
PZ C 2	-.03258	.02654	-.03084	-.23646	-.11955	.11434
S C 3	-.03277	-.01156	.00097	-.00942	.04323	.01649
PX C 3	.12945	.12453	.20783	-.11299	.06604	-.21064
PY C 3	.07071	.23314	.02937	.02172	.06334	.11173
PZ C 3	.13946	.02731	-.17974	-.05567	-.27252	-.09363
S C 4	-.02440	-.00222	.03252	-.02532	.01782	.02000
PX C 4	-.03654	.08372	-.00824	.08599	-.10787	.09715
PY C 4	.10500	.01314	-.07836	.15019	-.26519	-.18460
PZ C 4	-.09192	.02361	.03932	.16982	.14050	.11170
S H 5	.02791	-.05443	.01014	-.03811	-.00075	.03176
S H 6	.09970	.08914	.18427	-.11437	.10042	-.16366
S H 7	.07771	.07046	-.16640	.01076	-.15362	.04512
S C 8	-.01359	.03502	-.01263	-.02505	-.01641	.00498
PX C 8	-.12664	-.18303	-.18909	.13821	-.03269	.11162
PY C 8	-.01008	-.19465	-.12191	-.02117	.16363	.08392

PZ C 8	-.01010	.03550	-.03350	-.14474	-.15292	.06582
S H 9	.05987	.03370	-.04800	.13581	-.24779	-.11824
S H 10	.01329	-.07361	.02301	-.07685	.11113	-.06569
S C 11	.00950	.02659	-.01087	-.00368	-.07711	-.02948
PX C 11	-.08190	.07899	.11843	-.12878	.03438	-.33244
PY C 11	.09040	.24933	.14186	.03640	-.18549	-.01844
PZ C 11	.11077	.05576	-.22569	-.00830	-.15395	-.09147
S H 12	-.09061	-.15229	-.16467	.10157	-.02788	.11954
S H 13	.03296	-.02558	.02612	.03505	.18102	-.04599
S C 14	-.01810	.01369	.00614	-.01024	.00786	.00886
PX C 14	.01711	.13323	.10439	-.05929	-.05466	.05600
PY C 14	.10705	.08799	-.12116	.12432	-.08217	-.24247
PZ C 14	-.00685	.04321	.13733	.17598	-.00054	.10658
S H 15	-.12438	-.09514	.13233	-.04091	.15681	-.04220
S H 16	.07232	-.05589	-.11273	.11448	-.07001	.26178
S C 17	-.00405	.01957	.01469	-.00655	-.01235	.01900
PX C 17	-.01296	-.12833	-.09937	.05578	.04634	-.05049
PY C 17	.28991	-.19892	.06002	-.12440	.09332	.21527
1						
PZ C 17	-.19436	-.03002	-.10326	-.22501	.04655	-.05717
S C 18	.01462	-.02552	.05558	.00315	-.04543	.03498
PX C 18	.26477	-.05139	-.03731	.08511	.06876	.25382
PY C 18	-.19138	-.14074	.08910	-.15477	.07647	.10019
PZ C 18	-.04786	-.16183	.24261	.10260	-.25756	.04264
S C 19	-.02390	.01977	-.00703	.02699	.05135	.01056
PX C 19	-.01327	.09650	-.08900	.04287	.05339	.05748
PY C 19	-.07290	-.15299	.14613	-.07237	-.10793	.07201
PZ C 19	-.03802	-.23959	.19168	.02867	-.01304	-.07743

S C 20	-.01135	-.01969	.02935	.00837	.01484	-.00700
PX C 20	.28121	-.16440	.06568	-.17891	-.06303	-.04689
PY C 20	.17168	.10688	.04891	.19185	.17846	-.06810
PZ C 20	.10094	.19441	-.28145	-.17089	-.06379	.06698
S C 21	.04910	.00664	-.02808	.01586	.01861	-.01737
PX C 21	-.06805	.17698	.15495	.01323	-.07332	.12565
PY C 21	.10434	.00873	-.15088	.07133	.10742	-.15689
PZ C 21	-.00714	-.01711	.22440	.12933	-.18983	.04769
S H 22	-.03595	.08767	-.08263	.03431	.08014	.03805
S C 23	.00559	-.04530	.01002	-.00710	-.01053	.00647
PX C 23	.08794	-.20171	-.01928	-.05249	-.01982	-.23117
PY C 23	.12965	-.19258	.06194	.00326	-.15814	-.04327
PZ C 23	-.14495	.09134	-.09373	-.19301	.17450	-.00176
S H 24	.07927	-.14916	-.15368	-.01238	.07663	-.12595
S H 25	-.03578	.04203	.25065	.07032	-.20218	.13445
S H 26	.05478	-.19603	-.02246	-.05490	-.02733	-.22310
S H 27	-.12599	.19132	-.04015	.00917	.13544	.11279
S H 28	.21751	.03461	.06179	.11117	.12670	-.07862
S H 29	.07163	.03721	-.18322	-.25323	-.14148	.06615
S H 30	-.24304	.12484	-.03986	.15073	.05896	.04039
S H 31	-.25119	.02617	-.13205	-.09565	.00050	-.15787
S H 32	.22481	-.19572	.03448	-.08969	.08829	.18261
S H 33	.01802	.08481	.03353	.23163	-.06272	-.05267
S H 34	-.20907	.01940	.06595	-.07247	-.08735	-.20738
S H 35	.19189	.14384	-.18577	.02453	.15218	.02236

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ROOT NO.	31	32	33	34	35	36
	-12.26851	-12.04566	-11.89561	-11.78793	-11.52029	-11.39225
S O 1	-.07877	.06744	.02162	-.00771	.00412	.03997
PX O 1	.12876	-.18689	-.06565	.06246	-.10991	-.18069
PY O 1	-.20038	.18871	.06041	-.00180	-.00761	.09292
PZ O 1	-.02908	.17346	.02713	.40370	.45710	-.20879
S C 2	-.00380	.01985	-.00153	-.02203	.01650	.03671
PX C 2	-.11747	.13998	.04299	-.04376	.05566	.11545
PY C 2	.23855	-.07507	-.05030	.03589	.04672	-.05495
PZ C 2	-.05803	.05180	.01633	-.02219	-.03846	-.03837
S C 3	.04034	.01558	.00301	.01971	.02021	.00242
PX C 3	-.20755	-.13432	-.00692	-.10524	.03665	-.17306
PY C 3	-.09453	.10822	-.01104	.04665	-.07654	.06837
PZ C 3	-.04426	-.22884	.12568	-.12394	-.14003	.09844
S C 4	-.00034	.01173	.02219	.01259	-.01451	.02977
PX C 4	.28603	.18348	-.03828	.14326	-.07610	.26729
PY C 4	.00140	-.02501	-.18180	-.05647	.06911	-.05053
PZ C 4	-.06723	.25777	-.23192	.07671	.15441	-.14747
S H 5	.11713	-.07874	-.02595	-.00254	.02216	-.02922
S H 6	-.17088	-.11845	-.01036	-.07887	.04540	-.17308
S H 7	.02082	-.06645	.10932	-.02393	-.13195	.16444
S C 8	-.01334	-.00418	.00689	-.00408	-.02268	.04765
PX C 8	-.14617	-.06838	.05265	-.16424	.01360	-.29996
PY C 8	.25071	-.06263	.22141	.07959	-.00684	-.02593
PZ C 8	-.00560	-.14654	.22159	-.08759	-.21752	.16391

S H 9	.08730	.04152	-.16140	.00157	.02940	.06090
S H 10	-.25781	-.14935	.04969	-.12936	.05270	-.23555
S C 11	.00093	-.02388	-.01448	.00516	.03243	.01823
PX C 11	-.04711	-.12546	-.01337	.07492	.10314	.27154
PY C 11	-.15214	.13642	-.22504	-.05525	-.07182	.05241
PZ C 11	.01339	-.04979	-.12126	.04198	.18771	-.09261
S H 12	-.14940	-.06478	.05199	-.15318	-.00674	-.26318
S H 13	.15289	.10474	-.08533	.15761	.14890	-.00295
S C 14	.00412	.01905	.00506	.02458	.03788	.00585
PX C 14	.25208	.11508	.04292	-.08831	-.28028	-.24563
PY C 14	.16355	.00627	.00383	.03896	.09736	-.07221
PZ C 14	-.12155	.12003	.03481	-.06636	-.09734	.06249
S H 15	.03791	-.07222	.17608	.01528	-.06597	.15632
S H 16	.04236	.09221	.00460	-.08047	-.09153	-.25656
S C 17	.05401	.03199	.01212	-.01809	-.03508	-.02900
PX C 17	-.23781	-.11926	-.04222	.06417	.27695	.27547
PY C 17	.00128	.03695	-.03534	.09122	-.08209	.11537
1						
PZ C 17	.12304	-.06757	.02249	-.09410	.09590	.02046
S C 18	-.02397	-.02174	-.02041	.00819	.01463	.03081
PX C 18	-.05854	-.22627	-.10559	-.05222	.16710	.13176
PY C 18	-.21212	.06721	-.02270	.02356	-.05771	.12001
PZ C 18	.02602	-.16576	.15211	.14325	.05481	-.04485
S C 19	-.00507	.02335	.00434	-.01686	-.00354	.01583
PX C 19	-.01414	-.24460	-.14948	.34078	-.14961	-.08061
PY C 19	-.10826	.00394	-.28198	-.04170	-.10799	.04504
PZ C 19	.16252	-.05005	-.12209	-.08848	.06212	-.01086
S C 20	.01339	.01605	-.03485	-.04689	.01240	.00806

PX	C	20	.00507	.23873	.08181	-.16742	.12305	.01821
PY	C	20	.03000	.03895	.20632	.12510	.07353	-.07177
PZ	C	20	-.11412	.00475	.12992	.13197	-.05264	-.02030
S	C	21	.03620	.01239	.01028	-.04210	.03560	.00153
PX	C	21	.16957	-.02218	.08629	-.23634	.19061	.01645
PY	C	21	.05647	.10181	.31241	.02523	.08614	-.02852
PZ	C	21	-.13653	-.03530	.24281	.17816	-.00500	-.02117
S	H	22	-.01258	-.21962	-.14001	.30753	-.14059	-.07536
S	C	23	.03094	-.02363	-.02367	-.01813	.02648	.00444
PX	C	23	-.12029	.21271	.00946	.16269	-.20914	-.04919
PY	C	23	.15937	-.11000	-.19468	-.03673	.03279	-.03259
PZ	C	23	.04063	.15616	-.24845	-.23228	-.06873	.04470
S	H	24	-.12189	.02006	-.08357	.21492	-.16620	-.02819
S	H	25	-.05444	-.07154	.08187	.02293	.04292	.00396
S	H	26	-.08329	.17251	-.01116	.14416	-.18101	-.05310
S	H	27	-.08375	.01608	.16029	-.02993	.05688	.05047
S	H	28	.03656	.10634	.20147	.02638	.10541	-.04437
S	H	29	-.09289	.06897	.01312	-.03451	-.02817	.02909
S	H	30	.00288	-.20678	-.10315	.14592	-.10078	-.01984
S	H	31	.03928	-.09448	.01664	-.06874	.16720	.02934
S	H	32	-.06627	.00300	-.03685	.07438	-.00896	.14665
S	H	33	-.12516	.02328	-.00506	.03686	.01315	-.00762
S	H	34	.05116	.19221	.08435	.05393	-.17201	-.12356
S	H	35	.03870	.00958	-.15057	-.13507	.04786	.04841

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ROOT NO.	37	38	39	40	41	42
	-10.72342	-10.45765	2.96179	3.40776	3.48648	3.60302
S O 1	.04275	.00270	-.18197	.03549	-.01098	-.01247
PX O 1	-.05679	.00627	-.45715	-.00200	-.07282	-.01730
PY O 1	.09510	.00617	.28201	-.05065	.02846	.04056
PZ O 1	.01247	.46268	.00929	.03380	-.03958	.01396
S C 2	.00696	.00524	.31489	.04234	.19121	.39942
PX C 2	.05442	.00616	-.48806	.07910	.02460	.19627
PY C 2	-.34206	-.03662	.03106	-.33100	-.21163	.01910
PZ C 2	.00403	-.37294	-.04760	-.24688	.29630	-.10095
S C 3	-.02646	-.01816	-.06927	.08634	-.03520	-.14693
PX C 3	.02928	.01431	-.03970	-.04773	.02233	.15174
PY C 3	.33181	.00976	.17474	-.23353	-.09688	.29621
PZ C 3	-.02200	.16505	-.02915	-.06147	.13267	-.00240
S C 4	.02087	-.00776	-.04234	.00941	.04230	.01671
PX C 4	-.02073	-.04345	-.01696	-.01377	.04834	.04999
PY C 4	-.22041	.01286	.03968	-.07097	-.06352	.04883
PZ C 4	.03836	-.17152	-.05866	-.08842	.17169	.03180
S H 5	-.07798	-.00783	.28768	-.10934	-.00624	.04222
S H 6	.00851	-.00270	.15266	-.03551	.01071	-.03987
S H 7	.10396	.13702	-.03979	.10327	-.04490	.05137
S C 8	-.01116	.00422	.02155	.03536	.02115	-.00475
PX C 8	.01144	.04209	-.03300	-.04802	.01233	.02997
PY C 8	.24188	.01552	-.00901	-.19122	-.05196	.06317
PZ C 8	-.00298	.13861	-.00103	-.07997	.08495	.02582

S H 9	-.21202	-.00900	-.00222	.09417	.01247	-.10753
S H 10	.04173	.02875	-.00417	-.03031	.01152	.05366
S C 11	.00109	-.03820	-.04298	-.05154	.10537	.03855
PX C 11	.02578	-.06533	-.03906	-.05278	.11431	.08757
PY C 11	-.25503	.03886	.03064	-.13571	-.18587	.01812
PZ C 11	.06226	-.23407	-.06868	-.09501	.24375	-.02144
S H 12	.00024	.04738	.01687	.02311	-.04367	-.03317
S H 13	.10872	-.12665	-.04240	-.03093	.11533	.01028
S C 14	.01252	.03479	-.06746	-.03015	-.05922	-.18015
PX C 14	-.02611	-.03236	-.15084	-.05220	.10742	.27491
PY C 14	.32391	.09199	-.05993	-.33391	-.22595	-.00906
PZ C 14	.01978	.37660	-.13269	-.29149	.18329	-.26019
S H 15	.08277	.14682	.00588	-.11120	-.00914	-.09088
S H 16	-.02122	.01723	-.02930	-.00742	.02791	.07800
S C 17	-.00515	-.00995	.07853	.02295	-.01328	-.02581
PX C 17	.02099	.02064	-.21610	-.06339	.05583	.14005
PY C 17	-.06929	-.02537	-.01586	-.06150	-.04587	-.00602
1						
PZ C 17	-.00611	-.08727	-.02609	-.05624	.03587	-.05489
S C 18	-.03816	-.02211	-.03963	-.10439	.03032	.05325
PX C 18	-.05281	-.01796	-.02258	-.09981	.05021	.14273
PY C 18	-.31028	-.04116	-.04196	-.23361	-.20886	.16495
PZ C 18	.03331	-.14072	-.02000	-.13019	.20061	-.11282
S C 19	.01110	-.05149	-.02680	-.00566	-.10689	-.19944
PX C 19	-.04751	.09369	-.09808	.03292	.07847	.26716
PY C 19	.26585	-.09168	-.04861	-.22083	-.28417	.00061
PZ C 19	-.07484	.31050	.07471	-.12570	.33872	.06552
S C 20	.02043	.02670	-.02927	.08366	-.00631	.07642
PX C 20	.02936	.02094	-.02076	.07455	.00653	.11950

PY C 20	-.12046	-.05427	.02796	-.13507	-.04920	-.08372
PZ C 20	-.04250	-.17317	.04710	-.16277	.08056	-.11725
S C 21	-.02146	.01080	-.03826	-.00357	-.05080	.09540
PX C 21	-.01528	-.01966	-.01710	-.01950	-.00130	.16686
PY C 21	-.24464	.01934	-.05289	-.22278	-.12461	.12964
PZ C 21	.00904	-.13406	-.00164	-.14581	.14630	-.04686
S H 22	-.04059	.06462	.16567	-.03272	.00879	-.11880
S C 23	.02162	-.00432	.02444	-.00848	-.04138	-.01396
PX C 23	.01040	.02061	-.03674	-.02588	.04445	.08337
PY C 23	.19901	-.00433	.00866	-.08776	-.10469	.05533
PZ C 23	-.03161	.14945	-.01994	-.21463	.26548	-.12056
S H 24	-.00714	.03991	-.02164	-.01222	.05660	.10212
S H 25	.11172	-.13217	.01738	.03173	-.17997	-.04642
S H 26	.03453	.01679	.01738	.04521	-.00669	-.09348
S H 27	-.18926	-.00741	-.03593	-.11630	-.06408	.11757
S H 28	-.09383	-.01239	.01417	.04377	.06841	-.02957
S H 29	.05307	-.10361	.00359	-.03067	-.11712	-.05970
S H 30	-.01550	.01939	-.01759	.01044	.01927	.07635
S H 31	.03961	-.06486	.03160	.02323	-.07505	.03029
S H 32	-.07538	-.02171	.02642	.08149	.05128	-.01668
S H 33	.04857	.10151	-.05066	-.10259	.00377	-.08387
S H 34	.01902	-.00578	-.02887	-.00195	.02881	.11853
S H 35	.08581	.13162	.00402	-.13077	.02874	-.13392

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ROOT NO.	43	44	45	46	47	48
	3.75687	3.82183	4.05869	4.10359	4.20670	4.26398
S O 1	.02892	-.03430	-.01962	.01061	-.02778	.03555
PX O 1	.03401	-.01082	.00073	.01593	-.05647	.07492
PY O 1	-.05033	.06109	.03582	-.01522	.05192	-.06323
PZ O 1	-.02104	-.01204	-.00583	.03580	-.01372	-.01571
S C 2	.08445	-.10509	.01425	-.00437	-.05259	.06129
PX C 2	.13034	-.12734	-.03195	.03615	-.13268	.16621
PY C 2	-.02316	.16008	.11615	-.02204	-.10026	.11438
PZ C 2	.17172	.09887	.00595	-.26988	.13069	.14085
S C 3	-.09167	-.02178	-.02444	.05177	-.03830	.01410
PX C 3	.10742	-.04240	.01095	-.03776	.11721	.04303
PY C 3	-.01310	.03428	.10983	.05420	-.21101	.17597
PZ C 3	.18419	.09361	-.05116	-.19426	.06759	-.06523
S C 4	.08318	-.02745	.04617	-.05831	.23620	.01053
PX C 4	.06990	-.03500	.04562	-.08036	.29343	.01598
PY C 4	-.11302	.01455	-.05450	.03362	-.31897	.10580
PZ C 4	.18510	.11952	-.17895	-.21193	-.25190	-.06693
S H 5	-.06188	.09483	.06266	-.02325	.04136	-.05607
S H 6	-.04050	.07304	.00862	-.01544	-.08568	-.05752
S H 7	-.03743	-.11151	.02087	.09924	.13245	-.02445
S C 8	.08726	.06292	.00249	.00227	-.19879	-.02335
PX C 8	-.08793	-.06846	-.01507	-.03188	.29171	-.05560
PY C 8	-.20176	-.04048	-.14830	-.12002	-.16501	.16243
PZ C 8	.02934	.10291	-.16551	-.07017	-.37295	-.09102
S H 9	.02208	.02576	-.00202	.04984	.00912	-.12673

S H 10	.00169	-.02593	.00581	-.03373	.11185	.02072
S C 11	-.11016	-.00503	-.10230	.06044	.01806	-.02726
PX C 11	-.15091	-.04083	-.01750	.01448	.08341	-.11606
PY C 11	-.13974	-.08786	-.04688	-.17442	.02837	.25267
PZ C 11	-.07681	.12083	-.19668	.11537	-.10674	-.20217
S H 12	.02069	.01888	.01612	.02915	-.13787	.07800
S H 13	.02033	.03345	-.08706	-.01552	.05209	-.16795
S C 14	.03963	.11480	.41577	-.23887	-.02254	.11392
PX C 14	-.26330	-.12937	.21396	-.10817	-.11206	-.31018
PY C 14	-.07152	-.12394	-.16926	-.16460	.17529	.07284
PZ C 14	-.03137	.23980	-.07997	-.02827	.03776	-.18211
S H 15	.01147	.09838	-.10792	-.04293	-.13433	.01423
S H 16	-.08025	-.06153	.08699	-.04434	.08173	-.09273
S C 17	.06633	.01177	-.16141	.09367	.04481	.04867
PX C 17	-.20538	-.04004	.42289	-.22500	-.09635	-.17974
PY C 17	-.00568	-.05221	-.06771	-.07474	.08932	.01698
1						
PZ C 17	.00749	.08042	-.04705	.00946	.01184	-.04735
S C 18	-.16710	-.04845	-.12016	.09495	.05670	.09284
PX C 18	-.26000	.01798	.00896	.03760	.05023	-.02032
PY C 18	.00054	-.23567	-.34108	-.12461	.08088	-.13898
PZ C 18	-.21119	.03757	.01196	.26551	.07475	.14160
S C 19	-.14865	-.07551	.04021	.01219	-.06431	.17715
PX C 19	.15234	.18258	-.07111	.10525	.05431	.13998
PY C 19	.18684	.16245	.21264	.26673	.03617	-.12503
PZ C 19	.22854	-.15253	.12360	-.13968	.03572	.14125
S C 20	-.02675	.06235	-.07654	.00013	-.00023	-.04112
PX C 20	.00457	.09759	-.07789	.03558	.01844	.01736
PY C 20	.06080	.01611	.13727	.05674	.00125	.00578

PZ	C	20	.09629	-.14894	.15456	-.03917	-.01591	.13856
S	C	21	.05291	.21347	.04309	-.02349	.05509	.00173
PX	C	21	.01862	.29717	.03831	.05202	.12666	.13756
PY	C	21	.32131	.03112	.13311	.28858	.00233	-.21566
PZ	C	21	.10147	-.31805	.05396	.22406	-.07078	.05506
S	H	22	-.04252	-.12248	.04094	-.10889	-.00342	-.27525
S	C	23	.16497	-.18261	.03146	-.02999	-.07026	-.04327
PX	C	23	-.19478	.24559	-.02987	.07823	.13814	.02027
PY	C	23	.22944	-.22095	-.04300	.03342	-.03326	-.19592
PZ	C	23	-.11847	-.23630	.10854	.40574	-.04278	.05988
S	H	24	-.01899	.12475	-.00504	.08195	.07865	.14782
S	H	25	.02668	-.00518	-.03300	-.05002	-.03410	-.20451
S	H	26	.06446	-.10049	.00924	-.06043	-.08525	.01888
S	H	27	.01984	.02602	-.08583	.09335	.07890	-.14803
S	H	28	-.05309	-.11534	-.05063	-.07871	-.02518	.03070
S	H	29	-.04035	.06221	.03186	.05415	.00918	-.08583
S	H	30	.04362	.05755	-.01709	.03836	.01833	.06442
S	H	31	.01263	-.08857	-.01217	-.03311	.03889	.09664
S	H	32	.02585	.06047	.06312	.07398	-.08403	.00515
S	H	33	.00675	.05363	-.06405	-.04569	.04913	-.02319
S	H	34	-.13688	.05617	.11220	-.04530	-.00606	-.09535
S	H	35	.06438	-.06302	-.05950	.07323	.03851	-.02194

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ROOT NO.	49	50	51	52	53	54
	4.37894	4.42584	4.48113	4.54302	4.61770	4.82634
S O 1	.00346	.00069	-.02292	.03080	.04921	-.00428
PX O 1	.05733	.04792	-.06697	-.01174	.01243	-.03959
PY O 1	-.00117	.00349	.05152	-.06054	-.10211	-.00443
PZ O 1	.02425	-.01229	-.01256	.01882	-.03506	.00238
S C 2	.02600	.04612	-.07271	.00859	.06283	.03965
PX C 2	.08454	.07793	-.15571	.04577	.13816	-.03330
PY C 2	.23570	.19478	-.25868	-.20088	-.08721	-.08945
PZ C 2	-.19298	.11871	.09086	-.13377	.24676	-.02236
S C 3	-.19020	.02528	.07421	.05450	.09527	.02591
PX C 3	.24451	-.01380	-.21873	-.00999	-.07208	-.07888
PY C 3	.06026	.28106	-.18230	-.12455	.10011	.00373
PZ C 3	.21594	-.25796	-.00541	-.05886	-.15492	-.01427
S C 4	.05804	-.04870	-.06216	-.04306	-.03100	-.04783
PX C 4	.06917	-.07170	-.19199	-.05234	-.12083	-.09570
PY C 4	-.14943	.03787	-.08787	.03504	.06722	-.01709
PZ C 4	.24256	-.35976	.02971	.03761	-.15014	-.01069
S H 5	.03297	.03589	.01927	-.10947	-.14339	-.01150
S H 6	-.08217	-.01354	.16552	-.03950	-.01829	.06502
S H 7	.03608	.05963	-.05177	.06890	-.02572	-.02627
S C 8	.12108	.03537	.07287	-.02028	.02761	.05027
PX C 8	-.11455	-.05319	-.19976	.01870	-.17889	.00059
PY C 8	-.32479	-.30598	-.08932	.09372	-.02456	-.07541
PZ C 8	.10179	-.14937	.01522	.06845	-.10671	.06804
S H 9	.07509	.03041	.21097	.02102	.00536	.08526

S H 10	.01815	-.02811	-.16916	-.01279	-.09119	-.05957
S C 11	-.18743	-.00530	-.14232	.07101	-.01797	-.04460
PX C 11	-.21143	-.00770	-.16059	.04177	-.09486	.07223
PY C 11	-.27706	-.34274	-.08851	.04496	-.05569	-.12864
PZ C 11	-.08751	.15807	-.11766	.07864	-.04175	-.02044
S H 12	.02237	.03015	.14994	-.00542	.15699	-.03250
S H 13	.09837	-.02825	-.08497	.03669	-.16485	.04474
S C 14	-.05963	-.10478	.07372	-.17818	.02135	-.06642
PX C 14	-.01484	.04481	.10977	-.03340	-.06256	.14201
PY C 14	.15643	.02431	.26215	-.03249	.09024	.06559
PZ C 14	-.12365	.24021	-.10444	-.02771	-.02566	-.01456
S H 15	.03178	-.02352	.03664	.01611	-.01182	-.05822
S H 16	-.06096	-.01566	-.04411	-.01981	-.07601	.11418
S C 17	.01737	.02488	-.03321	.06441	-.03142	-.00468
PX C 17	-.04306	-.01752	.12963	-.11434	-.05536	.06338
PY C 17	.06759	-.00017	.07880	-.07221	.12800	.21158
1						
PZ C 17	-.04854	.17352	-.02996	-.00515	-.04579	-.17206
S C 18	.14202	-.04587	-.01411	.03961	.07164	.16831
PX C 18	.19132	-.02681	.11880	.16878	.03847	-.12224
PY C 18	.02148	.16294	.14209	.00793	-.02404	.11771
PZ C 18	.13145	-.15382	-.00819	-.14038	.09158	.19690
S C 19	.11990	.15370	.07448	.15638	-.41283	.03199
PX C 19	-.19795	.02216	.17054	-.19362	-.19860	.09601
PY C 19	-.03880	-.13658	-.02368	.27378	-.01008	.10198
PZ C 19	-.07836	.10570	.04212	.38691	.07655	.11744
S C 20	-.04039	-.03815	-.00874	-.13017	.09968	-.00523
PX C 20	-.11446	-.02160	.08035	-.16615	-.04091	.13813
PY C 20	.00247	-.01119	.00274	.25101	-.08898	.15606
PZ C 20	.01126	.11988	.05403	.38756	-.11029	.10082

S C 21	-.01161	-.04712	-.10205	.11988	.18301	.14451
PX C 21	-.02425	-.03059	.13077	.08297	.03412	-.06540
PY C 21	-.15425	-.19060	-.03539	-.04614	.08478	.06113
PZ C 21	-.00975	-.06438	.12761	-.17525	-.06319	-.21024
S H 22	.08587	-.12911	-.20860	.05379	.46235	-.11475
S C 23	-.06282	.05479	.06492	-.02308	-.10600	-.20633
PX C 23	.10238	-.04904	.12935	.16107	.13784	-.17464
PY C 23	-.12712	.03652	.17577	-.03645	-.05118	-.28660
PZ C 23	.11176	-.19848	.02777	-.15482	-.00210	-.02615
S H 24	-.01715	.00555	.20700	-.01092	-.09730	-.16898
S H 25	-.04969	.01455	-.07712	-.00897	-.07370	.08660
S H 26	-.05298	.01348	-.18429	-.13518	-.05807	.31974
S H 27	-.03147	-.02995	.15102	.03918	.08635	-.13420
S H 28	.06379	.05742	-.01938	-.08013	.02375	-.17627
S H 29	.06756	-.06716	-.06325	-.02944	-.01922	-.04421
S H 30	-.09173	.01286	.09082	-.04649	-.12204	.14942
S H 31	.07615	-.14737	.06522	-.02639	.11259	.19712
S H 32	-.06836	-.01441	-.10907	.05195	-.08556	-.20380
S H 33	-.01066	.13173	.00328	-.05606	.06114	-.05351
S H 34	.06653	.00713	.11951	.14161	-.00560	-.23896
S H 35	-.07199	-.00277	.03007	-.19729	-.01300	.10124

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ROOT NO.	55	56	57	58	59	60
	4.99318	5.05573	5.10149	5.13069	5.15175	5.21729
S O 1	.00064	-.00260	-.02569	-.03622	-.00348	-.00889
PX O 1	.00300	-.02666	-.00805	-.05182	-.01051	.01617
PY O 1	.00009	-.00092	.06371	.07949	.00995	.02443
PZ O 1	-.00457	.00754	-.00353	-.00815	.00911	.00785
S C 2	.02462	.04019	-.04222	.02931	.03265	-.01824
PX C 2	.01777	-.01146	-.08195	-.11234	-.00052	-.00378
PY C 2	.02534	-.06683	-.01319	-.09333	-.02204	.05171
PZ C 2	.04026	-.07334	.05574	.03477	-.10134	-.04957
S C 3	-.09694	-.02994	.14758	.04766	-.05417	-.14145
PX C 3	-.00671	-.02864	.21323	.34930	.03526	-.04711
PY C 3	.00137	-.03891	-.05969	-.15833	-.04538	-.00600
PZ C 3	.11521	.04805	-.16236	-.20707	-.00263	-.02432
S C 4	.13245	.02302	-.12710	-.07237	.00051	.03679
PX C 4	.01233	.00326	.08434	.02904	-.01526	-.10922
PY C 4	-.19193	-.02226	.17290	-.02359	.01633	-.20562
PZ C 4	-.01436	.05710	.00168	.03194	.10213	-.03472
S H 5	.00548	-.00974	.07182	.08187	.00831	.04519
S H 6	.06707	.04865	-.28538	-.33588	.00258	.14201
S H 7	-.00817	-.00063	.09291	.28417	.06278	.09646
S C 8	-.15509	.02993	.09204	-.08410	.04123	-.14275
PX C 8	-.15616	-.01109	.02266	-.16651	-.07021	.04559
PY C 8	.04807	.07037	-.03891	.04626	.05418	.03736
PZ C 8	-.20718	-.03566	.09586	-.03236	.03295	-.05121
S H 9	.05700	.00014	-.07288	.06410	-.00944	.16977
S H 10	-.10259	-.01695	.18711	.08341	-.01643	-.13741

S C 11	.06471	.03080	-.07401	-.00663	.01587	.01492
PX C 11	-.12410	-.02311	-.09521	-.20589	.04112	-.02863
PY C 11	.08099	.04124	.00832	.10985	-.02255	.12934
PZ C 11	.05333	-.07265	.04679	.20434	-.14893	.19595
S H 12	.24480	.00372	-.07840	.21418	.03308	.06664
S H 13	-.10200	-.08043	.01958	-.03271	-.05173	.07061
S C 14	-.03170	-.02230	.08480	.00428	.01949	-.02899
PX C 14	.01006	-.02848	-.06455	.16349	.09318	.03725
PY C 14	.12689	-.02678	-.07655	.01341	.00374	-.07630
PZ C 14	-.01620	-.14763	.01527	-.02878	-.16398	.07306
S H 15	.06261	-.05465	.11996	.25434	-.13992	.18429
S H 16	-.17086	-.04285	-.03831	-.19152	.03462	-.04054
S C 17	-.01142	.00784	.01019	.00722	.01260	-.02297
PX C 17	-.01683	-.00419	.00420	.13414	.10388	-.00559
PY C 17	-.33784	.26902	.21127	-.03605	-.11426	.14613
1						
PZ C 17	.01696	.52080	-.08191	.06261	.27982	-.09511
S C 18	.01012	.07027	-.10630	.01280	.03050	.09184
PX C 18	.18841	.16032	.09860	-.08830	-.30867	.03429
PY C 18	.04795	-.09047	-.12909	.09612	.09438	-.07169
PZ C 18	.07725	-.08866	.03614	.02738	.25706	-.15057
S C 19	-.00419	-.02498	.01041	-.04230	.02074	-.02247
PX C 19	.08966	.03493	.04217	.02418	-.04975	.05285
PY C 19	-.02579	.02945	.02274	-.00021	.10217	.18360
PZ C 19	.01133	-.02024	-.02286	.03660	.03865	-.06255
S C 20	.01335	.00839	.01516	-.02836	-.00904	-.01505
PX C 20	.15113	.10503	.19409	-.04045	-.11661	-.18058
PY C 20	-.07032	.05766	-.22166	.14899	-.23918	-.38499
PZ C 20	.07723	-.01617	.21064	-.13387	.18923	.13223

S C 21	.05577	.04580	-.07153	.01052	-.04549	.03254
PX C 21	-.29178	-.09323	-.17667	.13734	.10217	.15063
PY C 21	.08401	.08783	.11207	-.00791	.02255	.11528
PZ C 21	-.16076	.05497	-.13744	.04031	-.18253	.04038
S H 22	-.06149	-.00789	-.04027	.01757	.03448	-.03434
S C 23	-.10009	.07321	.00426	.00001	-.08312	.00399
PX C 23	-.02387	-.08693	.12775	-.12710	.16706	-.17308
PY C 23	-.05590	-.12057	.06438	-.08381	-.01878	-.08952
PZ C 23	.06565	.09919	.07513	-.05156	-.04928	.00959
S H 24	-.29552	-.11171	-.10739	.10020	.11556	.09651
S H 25	.19271	-.00898	.24434	-.07986	.13511	-.04695
S H 26	.09924	.03981	-.11472	.11421	-.06403	.13527
S H 27	.02265	-.17197	.08252	-.10003	.09124	-.11715
S H 28	.00092	-.08826	.11327	-.10600	.23266	.36525
S H 29	-.14318	-.00115	-.31153	.18782	-.19139	-.18458
S H 30	.13807	.09251	.16714	-.02139	-.09917	-.15349
S H 31	-.14215	-.25351	.14212	-.10463	-.27309	.13468
S H 32	.28206	-.22138	-.16633	-.01227	.05549	-.11121
S H 33	-.11911	.48551	.01768	-.01144	.11772	.00886
S H 34	.15656	.08830	.15241	-.08857	-.28046	-.03749
S H 35	.00935	-.20073	.02144	.06986	.27493	-.20322

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ROOT NO.	61	62	63	64	65	66
	5.29692	5.36110	5.38222	5.46573	5.51069	5.53815
S O 1	.00399	.00138	.00942	.02922	-.01226	-.00190
PX O 1	-.00915	-.00995	.04403	.01399	.04614	.02384
PY O 1	-.02301	-.02642	.00104	-.07009	.04768	.01552
PZ O 1	-.00803	.00790	.00515	-.00477	-.00368	-.00857
S C 2	-.05108	-.00176	-.02442	.11666	.02611	-.02336
PX C 2	-.02936	-.01519	.06388	.14388	.05352	.01756
PY C 2	-.03329	.10466	.05515	.03233	.12125	.03622
PZ C 2	.07330	-.13062	-.09250	.03136	.07517	.00362
S C 3	.01155	-.02067	.02573	-.16664	-.06935	-.22988
PX C 3	-.05395	.04537	.01649	-.13971	.24076	-.07627
PY C 3	-.02811	.04988	.05761	.10155	.05892	-.13207
PZ C 3	-.16038	.12188	.12534	-.06832	-.14430	-.15144
S C 4	-.13933	.05998	.04804	-.00584	-.12631	.19295
PX C 4	-.04007	.03130	-.02337	-.07241	-.33691	.03581
PY C 4	.05828	-.10324	-.09963	-.11900	-.29434	.21486
PZ C 4	-.04847	-.00392	-.00770	-.10074	.07039	.00161
S H 5	-.02800	-.01048	-.00254	-.07963	.07850	.02628
S H 6	.02261	-.01798	-.02829	.22810	-.14870	.20251
S H 7	.10116	-.06008	-.10671	.09200	.18852	.29201
S C 8	.07621	-.08504	-.06003	-.05025	-.07198	-.28700
PX C 8	.23839	-.04225	-.04653	.27647	.00576	-.06865
PY C 8	-.14155	.03054	.04314	-.07563	.14759	-.11841
PZ C 8	.21024	-.09380	-.07711	.03225	.12222	.21060
S H 9	.06763	.02756	.04899	.11321	.39932	-.30305
S H 10	.07659	-.01988	-.05978	-.05572	-.20678	-.10811

S C 11	-.17044	.03757	.06060	-.12111	-.01473	.15218
PX C 11	-.10128	-.02188	.06028	-.23776	.27421	-.06366
PY C 11	.02692	.05531	.00098	.22033	.08117	-.00622
PZ C 11	-.09144	.12580	.06398	.16655	-.14054	-.10796
S H 12	-.26207	.09843	.08252	-.18253	.03944	.24557
S H 13	.21225	-.02495	-.03719	.16539	.07514	.35665
S C 14	.05510	.01281	-.07062	.05720	.05255	.03121
PX C 14	-.03117	.08863	.02295	.01636	-.12792	.02293
PY C 14	.22451	-.12124	-.05143	-.08761	-.06744	-.05283
PZ C 14	-.09012	.02990	.05405	-.17014	.01198	.02187
S H 15	.10248	.08539	-.01874	.33612	-.12854	-.16347
S H 16	.04542	-.04605	.00304	-.10884	.24124	-.15789
S C 17	-.02659	-.01741	.05112	.03634	-.10502	-.18031
PX C 17	.00087	.06149	-.00157	.06955	-.11465	-.06197
PY C 17	-.28622	.07453	.00505	.05244	.02142	.08103
1						
PZ C 17	.09478	.00528	-.06996	.03357	.02957	-.01502
S C 18	.08125	.16414	-.11627	-.00843	-.12389	-.10585
PX C 18	.05948	-.21975	-.03342	-.14593	-.00458	-.00083
PY C 18	.06941	-.13917	.14389	-.04510	-.04351	.01551
PZ C 18	-.02260	-.10829	.01485	.09366	.03793	.04243
S C 19	-.11320	.06477	-.05928	-.00794	.00318	.00550
PX C 19	-.07446	-.19981	-.23188	.01111	.00079	-.05164
PY C 19	.06731	-.02742	.00559	-.12118	-.05742	-.00182
PZ C 19	-.08939	-.08910	-.09150	.10479	.01379	-.00443
S C 20	.05386	.03348	.07248	-.00625	-.03211	-.02392
PX C 20	.21241	.29311	.28507	-.01394	.05126	.08506
PY C 20	-.10734	.05947	.02839	.13598	.03735	.02557
PZ C 20	.09177	.15080	.12646	-.07126	-.03219	.02575
S C 21	.16476	.05349	-.15345	-.09038	.05409	.00401

PX C 21	.10474	.02171	.17180	-.13649	-.08394	.03045
PY C 21	-.01983	-.19832	.05629	.02128	-.05823	-.03516
PZ C 21	.16256	.11977	.03059	-.12191	.02267	.01464
S H 22	.13483	.09956	.20766	-.00195	-.00731	.01875
S C 23	-.01399	-.17079	.33184	.09590	.00840	-.00636
PX C 23	-.11613	.09307	-.00377	.21877	.06676	-.01224
PY C 23	-.08150	.28362	-.23805	-.00146	.05736	.01815
PZ C 23	-.01684	-.01744	-.03671	.03600	-.03191	-.03922
S H 24	-.02894	-.01556	.23644	-.03586	-.10641	.01684
S H 25	-.25487	-.19049	.06542	.17942	-.04938	-.03096
S H 26	.10608	.04140	-.22705	-.23044	-.06365	.00348
S H 27	-.08064	.34821	-.40097	-.00989	.05092	.01323
S H 28	-.01726	-.14953	-.14575	-.09875	-.02910	-.04319
S H 29	-.19678	-.17598	-.20005	.10258	.04298	-.01264
S H 30	.14799	.23191	.19109	-.00571	.06443	.08576
S H 31	-.16591	.00670	.01993	-.03202	.09250	.17158
S H 32	.24528	-.06308	-.03864	-.08497	.08469	.04429
S H 33	-.02775	.03262	-.08074	-.00159	.12036	.15260
S H 34	-.00891	-.27815	.05068	-.09867	.07338	.07155
S H 35	-.06563	-.17631	.15585	.08301	.09248	.10381

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ROOT NO.	67	68	69	70	71	72

	5.56531	5.67080	5.69154	5.82303	5.87477	5.98148
S O 1	.00057	-.00891	.00751	.00607	-.01170	.01663
PX O 1	-.00186	-.06906	-.04329	-.07171	.02250	-.03711
PY O 1	-.00531	-.02568	-.02831	-.04762	.03078	-.06323
PZ O 1	.02293	-.00842	.00326	.01895	.00007	-.01139
S C 2	.00527	-.01848	.03888	.03182	-.00613	.02278
PX C 2	.00207	-.12502	-.03403	-.06954	.00330	.00234
PY C 2	.00609	.01131	-.03778	-.07587	-.02257	-.02751
PZ C 2	-.13554	.06000	-.03495	-.07851	-.02367	-.02640
S C 3	-.04045	.02278	.30899	.17491	-.01099	.07217
PX C 3	-.04698	.05918	.02857	.01497	-.10036	-.00661
PY C 3	-.00720	-.04154	.19722	.04473	.02525	.04818
PZ C 3	.04796	-.04134	.15894	.13872	-.00465	.04886
S C 4	.02223	.05388	-.09516	.10931	-.28124	.01884
PX C 4	.05241	-.03618	-.06003	.04773	.21232	-.03431
PY C 4	-.00953	.06918	-.10561	.08430	-.11893	.00260
PZ C 4	.01943	-.00234	-.18255	-.10280	.01302	-.03303
S H 5	-.00151	-.02193	-.05276	-.08295	.06084	-.09883
S H 6	.07222	-.05203	-.22068	-.13549	.06439	-.04427
S H 7	-.01556	.03272	-.37177	-.21130	-.02664	-.11973
S C 8	.06475	-.10368	-.27840	-.15017	.05607	.00758
PX C 8	.02795	-.07934	.11559	-.11319	-.02063	.04366
PY C 8	.04096	-.03705	-.07727	-.15543	.09095	-.01113
PZ C 8	-.09508	.08470	.21268	-.00784	-.01691	-.00800
S H 9	-.02274	-.07640	.15362	-.14069	.21003	-.00548
S H 10	.02808	-.06852	.02578	-.04166	.36757	-.03662
S C 11	.01582	.03340	.20085	-.33354	.19209	.01194

PX C 11	-.05175	.07490	-.15442	.15537	-.12644	-.03589
PY C 11	.02643	-.04091	.06901	.09290	-.06447	.00385
PZ C 11	.10714	-.08269	-.13180	.16550	-.02001	.01690
S H 12	-.05906	.14161	.11123	.17265	-.04141	-.03710
S H 13	-.11009	.11242	.37471	.11601	-.08259	.00531
S C 14	-.03272	.02438	.02354	-.01761	-.02033	-.01113
PX C 14	.01722	-.00366	.01431	.05978	.16582	.02765
PY C 14	-.15034	.08647	-.03002	.00902	.00490	-.01433
PZ C 14	-.03815	.09018	-.05834	-.11586	.04887	-.02141
S H 15	.07596	-.10162	-.15277	.30386	-.12866	.01082
S H 16	-.06120	.04022	-.26221	.35064	-.23109	-.03322
S C 17	.09788	.20755	.07095	-.28177	-.35523	-.04551
PX C 17	.05139	.11594	.06348	-.11721	-.10721	-.01330
PY C 17	.10953	-.05407	.03380	-.01582	-.00543	.00477
1						
PZ C 17	-.00914	-.05951	.04669	.08828	-.04196	.01283
S C 18	-.31930	.21583	-.06012	-.00039	.08666	-.02297
PX C 18	-.00742	-.15336	.02575	-.04284	-.11701	.01160
PY C 18	.12910	-.02029	-.00109	.04578	.04776	.01418
PZ C 18	.17622	-.14476	.04008	.03703	-.03963	.02701
S C 19	.04557	.00526	.01069	.02830	.01528	-.01200
PX C 19	.03223	.12363	.04077	.06387	.04148	-.10523
PY C 19	.12211	.04586	.00823	.03929	.03563	.06990
PZ C 19	-.05098	-.03712	-.00067	-.00553	.00808	.10619
S C 20	-.02142	-.08953	.07547	.03666	-.02083	-.56515
PX C 20	-.03575	-.00775	-.08687	-.06320	-.02283	.14926
PY C 20	-.07107	-.07778	-.00735	-.01049	-.01055	-.11126
PZ C 20	.04107	-.06125	.01096	.01176	-.00057	-.13943
S C 21	.36074	.18180	.00872	.06021	.07631	-.02574
PX C 21	-.06359	-.20958	.01652	-.03819	-.06999	.07416

PY C 21	-.14560	.03347	-.00523	.00476	.00819	.01013
PZ C 21	.18987	.09416	-.00083	.02074	.03062	-.05283
S H 22	-.04716	-.07038	-.02662	-.06512	-.04922	.06848
S C 23	.02142	.25882	-.05146	.05895	.12691	-.04247
PX C 23	.03872	.23596	-.03956	.05875	.10857	-.02385
PY C 23	.00254	-.10415	.02354	-.04262	-.06826	-.00016
PZ C 23	-.18491	.02014	-.01159	-.01376	-.01539	-.01798
S H 24	-.28930	-.26644	.00997	-.05893	-.09887	.06391
S H 25	-.39011	-.11341	-.01067	-.03951	-.04705	.02423
S H 26	-.03732	-.33423	.06832	-.09006	-.17444	.04169
S H 27	-.00349	-.18114	.03911	-.05112	-.09885	.02162
S H 28	.07392	.11387	.00089	.01034	.02729	.39881
S H 29	-.02261	.07046	-.03581	-.01758	.01599	.35303
S H 30	-.00962	.05595	-.11761	-.07048	-.00366	.47683
S H 31	-.02837	-.12416	-.08059	.16070	.28325	.02297
S H 32	-.15344	-.13395	-.08090	.21641	.25311	.03328
S H 33	-.04845	-.20869	-.01655	.24265	.22202	.03924
S H 34	.20972	-.24706	.06463	-.02751	-.13351	.02803
S H 35	.36879	-.19349	.05942	.03821	-.03676	.03054

1

ROOT NO.	73	74

6.08479 6.27518

S	O	1	-.00623	.08148
PX	O	1	-.08501	-.37405
PY	O	1	-.01488	-.45734
PZ	O	1	-.00534	-.00033
S	C	2	.02128	.11017
PX	C	2	-.13321	-.30048
PY	C	2	.00381	.18417
PZ	C	2	-.02409	.01024
S	C	3	.08794	-.11842
PX	C	3	.19669	.06839
PY	C	3	-.03012	.02316
PZ	C	3	.05182	-.05180
S	C	4	.29509	-.07011
PX	C	4	-.32102	.05200
PY	C	4	.07675	-.05402
PZ	C	4	.03448	.05125
S	H	5	-.03736	-.62558
S	H	6	-.19046	.03135
S	H	7	-.02810	.11669
S	C	8	.19052	.01042
PX	C	8	.24483	-.03933
PY	C	8	.02609	.03397
PZ	C	8	-.09380	.00256
S	H	9	-.15951	.06449
S	H	10	-.43929	.09964
S	C	11	.14822	.02566
PX	C	11	-.19326	.03264

PY C 11 -.05886 -.02549
PZ C 11 .01025 -.01211

S H 12 -.29927 .01904

S H 13 -.11892 -.02440

S C 14 .00539 .03619
PX C 14 .12858 .02198
PY C 14 .01135 -.00659
PZ C 14 .04218 .07701

S H 15 -.06376 -.03762

S H 16 -.23156 .01183

S C 17 -.18545 -.01346
PX C 17 -.02763 .02064
PY C 17 -.01336 .01452
1
PZ C 17 -.02724 -.01024

S C 18 .03689 -.04305
PX C 18 -.04322 .02799
PY C 18 .02655 .00583
PZ C 18 -.01849 .00883

S C 19 .02468 .03967
PX C 19 .04684 .04310
PY C 19 .01229 -.00742
PZ C 19 -.03032 -.07187

S C 20 .06185 .04878
PX C 20 -.02563 .00808
PY C 20 .00072 -.01436
PZ C 20 .01854 .01065

S C 21 .02240 -.03861
PX C 21 -.02286 .02100
PY C 21 .00159 .00896

PZ	C	21	.01903	-.00875
S	H	22	-.04692	-.04487
S	C	23	.04327	-.00028
PX	C	23	.02702	-.02834
PY	C	23	-.02353	.00540
PZ	C	23	-.00341	.00039
S	H	24	-.02516	.07464
S	H	25	-.01783	.02715
S	H	26	-.05298	.01812
S	H	27	-.03524	-.00294
S	H	28	-.03197	-.02728
S	H	29	-.04134	-.04144
S	H	30	-.05701	-.01818
S	H	31	.13459	.01361
S	H	32	.15342	-.00795
S	H	33	.10166	.00334
S	H	34	-.04568	.08154
S	H	35	-.01595	.02720

NET ATOMIC CHARGES AND DIPOLE CONTRIBUTIONS

ATOM NO.	TYPE	CHARGE	ATOM ELECTRON DENSITY
1	O	-.3536	6.3536
2	C	.0958	3.9042
3	C	-.1302	4.1302

4	C	-.1454	4.1454
5	H	.1973	.8027
6	H	.0822	.9178
7	H	.0873	.9127
8	C	-.1522	4.1522
9	H	.0722	.9278
10	H	.0941	.9059
11	C	-.1350	4.1350
12	H	.0741	.9259
13	H	.0762	.9238
14	C	-.0800	4.0800
15	H	.0736	.9264
16	H	.0889	.9111
17	C	-.1828	4.1828
18	C	-.1448	4.1448
19	C	-.1308	4.1308
20	C	-.1875	4.1875
21	C	-.1486	4.1486
22	H	.0989	.9011
23	C	-.1566	4.1566
24	H	.0770	.9230
25	H	.0805	.9195
26	H	.0810	.9190
27	H	.0771	.9229
28	H	.0716	.9284
29	H	.0651	.9349
30	H	.0809	.9191
31	H	.0702	.9298
32	H	.0738	.9262
33	H	.0722	.9278
34	H	.0767	.9233
35	H	.0810	.9190

DIPOLE	X	Y	Z	TOTAL
POINT-CHG.	1.286	-.371	-.017	1.339
HYBRID	.008	-.725	-.001	.725
SUM	1.294	-1.096	-.018	1.696

CARTESIAN COORDINATES

NO.	ATOM	X	Y	Z
1	O	.0000	.0000	.0000
2	C	1.5488	.0000	.0000
3	C	2.0443	1.4674	.0000
4	C	1.5031	2.1978	-1.2549
5	H	-.3433	-.9256	-.0030
6	H	3.0442	1.4811	-.0121
7	H	1.7141	1.9301	.8228
8	C	2.0100	1.4768	-2.5288
9	H	1.8272	3.1438	-1.2558
10	H	.5033	2.1875	-1.2414
11	C	1.5189	.0077	-2.5286
12	H	3.0097	1.4928	-2.5440
13	H	1.6564	1.9452	-3.3384
14	C	2.0685	-.7296	-1.2862
15	H	1.8430	-.4503	-3.3564
16	H	.5192	-.0078	-2.5081
17	C	3.6309	-.7397	-1.3549
18	C	1.5549	-2.1890	-1.2731
19	C	2.0568	-.7356	1.2768
20	C	1.5230	-.0198	2.5323
21	C	1.5468	-2.1991	1.2656
22	H	3.1540	-.7335	1.3011
23	C	2.0735	-2.9181	-.0047
24	H	.5469	-2.2040	1.2612
25	H	1.8794	-2.6744	2.0801
26	H	3.0735	-2.9080	-.0013
27	H	1.7492	-3.8640	-.0093
28	H	1.8504	.9250	2.5425
29	H	1.8488	-.4937	3.3506
30	H	.5232	-.0255	2.5202
31	H	3.9971	-1.2149	-.5549
32	H	3.9705	.2008	-1.3679
33	H	3.9255	-1.2116	-2.1860
34	H	.5549	-2.1887	-1.2701
35	H	1.8862	-2.6646	-2.0880

ATOMIC ORBITAL ELECTRON POPULATIONS

1.89286 1.18697 1.29278 1.98099 1.24801 .79474 .94564 .91579
1.19363 1.00448 .93485 .99723 1.19406 1.02999 .98411 .93721
.80269 .91782 .91274 1.19470 1.01342 .95827 .98578 .92778
.90590 1.19372 1.02210 .95376 .96541 .92593 .92380 1.22861
.95574 .94264 .95299 .92640 .91112 1.18421 .94229 1.02920
1.02713 1.19553 1.01190 .95197 .98542 1.22765 1.00762 .94572
.94983 1.17998 1.03128 1.00936 .96687 1.19584 1.01418 .95463
.98391 .90113 1.19640 1.02011 .99355 .94653 .92297 .91949
.91902 .92295 .92844 .93491 .91915 .92978 .92620 .92785
.92335 .91897
.ARC FILE OPENED
TOTAL CPU TIME .17 SECONDS

== MOPAC DONE ==

From the output, identify the number of occupied levels. The atomic orbital coefficients of the HOMO are then given by the eigenvector with that number on the line "Root No." in the "EIGENVECTORS" array. The LUMO is the next higher eigenvector. For example, geosmin ($C_{12}H_{22}O$) is being calculated, then there are 38 doubly occupied levels. The 38^{th} eigenvector is the HOMO and the 39^{th} eigenvector is the LUMO.

APPENDIX B ESTIMATION PROGRAM INTERFACE SUITE (EPI SUITE)

Overview of EPI SUITE

The Estimations Programs Interface for Windows (EPI Suite) is an interface program. The EPI suite of physical/chemical property and environmental fate estimation programs is developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC). EPI Suite estimates physical-chemical properties as well as the fate and transports of these chemicals with accuracy sufficient to support regulatory the screening applications (U.S. EPA). It transfers a single simplified molecular input line entry specification (SMILES) to thirteen separate structure estimation programs that require SMILES notations (The EPI Suite also has Name Lookup feature). EPI Suite is a screening-level tool and should not be used if acceptable measured values are available. A clear understanding of the estimation methods and their appropriate application is very important. The EPI Suite provides 3 types of results

1. Physical/Chemical (P/Chem.) properties.
2. Environmental fate properties.
3. Advanced environmental fate models.

The program's graphical user interfaced runs each of the thirteen separate programs included in the suite and displays resulting information. The thirteen stand-alone programs that are part of the EPI Suite of Programs are

1. **AOPWIN** – estimates atmospheric oxidation rates.
2. **BCFBAF** - estimates bioconcentration factor (BCF) and biotransformation rate (kM).

3. **BioHCwin** - estimates biodegradation of hydrocarbons.
4. **BIOWIN** - estimates biodegradation probability.
5. **ECOSAR** - estimates aquatic toxicity (LD50, LC50).
6. **HENRYWIN** - estimates Henry's law constant.
7. **HYDROWIN** - estimates aqueous hydrolysis rates (acid-, base-catalyzed).
8. **KOAWIN** - estimates octanol-air partition coefficient.
9. **KOCWIN** - estimates soil sorption coefficient (K_{OC}).
10. **KOWWIN** - estimates octanol-water partition coefficient.
11. **MPBPVP** - estimates melting point, boiling point, and vapor pressure (also referred to as MPBPWIN).
12. **WSKOWWIN** - estimates water solubility (from log octanol-water partition coefficient).
13. **WATERNT** - estimates water solubility (using atom-fragment methodology).

The EPI Suite Interface program is a convenience for users because it automatically executes each program in succession without user interaction. Also, the interface program executes four program models that cannot be run separately (they must be run using the interface); these programs are

1. **WVOLWIN** - Volatilization Rate from Water Model.
2. **STPWIN** – Sewage Treatment Plant Mode.
3. **AEROWIN** - Sorption to atmospheric particulates.
4. **LEVEL3NT** –Level III Fugacity Model.

Molecular Weight, Henry's Law Constant, log octanol-water partition coefficient and other parameters are transferred to these models and allow program execution (they require execution of the stand-alone individual programs).The EPI Interface can also start the Dermal Permeability Program (**DERMWIN**). DERMWIN must be run as a stand-alone program since the EPI Suite interface does not capture its output.

Individual estimation programs and/or their underlying predictive methods and equations have been described in numerous journal articles in peer-reviewed technical journals. The full reference citations are given in the Help files for the individual programs. In addition, EPI Suite™ has undergone detailed review by a panel of EPA's independent Science Advisory Board (SAB) (http//yosemite.epa.gov/sab/sabpeople.nsf/WebCommittees/BOARD), and the September 2007 report can be downloaded from

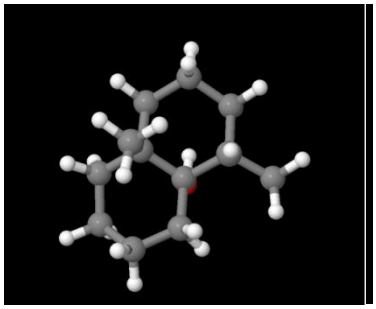
http//www.epa.gov/sab/panels/epi_suite_review_panel.htm.

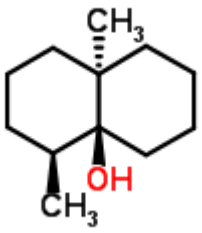
The properties of geosmin, 2-Metylisoborneol, acetaminophen, 2, 4 –Dichlorophenol, triclosan and atrazine were found using the EPI Suite v. 4.00.

Properties of Geosmin

Empirical Formula	$C_{12}H_{22}O$
Molecular Weight	182.3025
Nominal Mass	182 Da
Average Mass	182.3025 Da
Monoisotopic Mass	182.167065 Da

Structure of Geosmin





EPI SUMMARY

1. **Log Octanol-Water Partition Coef (SRC) (KOWWIN v1.67 estimate)**
   Log Kow = 3.57

2. **Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.42)**

Property	Temperature	Note
Boiling Point	248.80^{0}C	(Adapted Stein & Brown method)
Melting Point	47.08^{0}C	(Mean or Weighted MP)
Vapor Pressure(mm Hg,25^{0}C)	0.00057 mm Hg	(Modified Grain method)
Boiling Point (exp database)	270^{0}C	
Subcooled liquid Vapor Pressure	0.000907 mm Hg	(25 ^{0}C , Mod-Grain method)

3. **Water Solubility Estimate from Log Kow (WSKOW v1.41)**
   Water Solubility at 25 deg C (mg/L) = 156.7
   Water Sol Estimate from Fragments
   Water Sol (v1.01 est.) = 294.88 mg/L

4. **ECOSAR Class Program (ECOSAR v1.00)**
   Class/es found Neutral Organics

5. **Henrys Law Constant (25 deg C) [HENRYWIN v3.10]**
   Bond Method = 1.18E-005 atm-m^3/mole
   Group Method = 3.15E-006 atm-m^3/mole
   Henrys LC [VP/WSol estimate using EPI values] = 8.726E-007 atm-m^3/mole

6. **Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]**
   Log Kow used = 3.57 (KowWin EST.)
   Log Kaw used = -3.317 (HenryWin EST.)

Log Koa (KOAWIN v1.10 estimate) = 6.887
Log Koa (experimental database) = none

7. Probability of Rapid Biodegradation (BIOWIN v4.10)

- Rapid Probability Models
  Biowin1 (Linear Model) = 0.2929
  Biowin2 (Non-Linear Model) = 0.0462
- Expert Survey Biodegradation Results
  Biowin3 (Ultimate Survey Model) = 2.3721 (weeks-months)
  Biowin4 (Primary Survey Model) = 3.2778 (days-weeks)
- MITI Biodegradation Probability
  Biowin5 (MITI Linear Model) = 0.4564
  Biowin6 (MITI Non-Linear Model) = 0.4075
- Anaerobic Biodegradation Probability
  Biowin7 (Anaerobic Linear Model) = -0.7922

Ready Biodegradability Prediction NO

8. Hydrocarbon Biodegradation (BioHCwin v1.01)

Structure incompatible with current estimation method!

9. Sorption to aerosols (25 Dec C)[AEROWIN v1.00]

Vapor pressure (liquid/subcooled) = 0.121 Pa (0.000907 mm Hg)
Log Koa (Koawin EST) = 6.887
Kp (particle/gas partition coef. (m^3/ug))
Mackay model = 2.48E-005
Octanol/air (Koa) model = 1.89E-006
Fraction sorbed to airborne particulates (phi)
Junge-Pankow model = 0.000895
Mackay model = 0.00198
Octanol/air (Koa) model = 0.000151

10. Atmospheric Oxidation (25 deg C) [AopWin v1.92]

- Hydroxyl Radicals Reaction
  OVERALL OH Rate Constant = 22.3859 E-12 cm^3/molecule-sec
  Half-Life = 0.478 Days (12-hr day; 1.5E6 OH/cm^3)
  Half-Life = 5.734 Hrs
- Ozone Reaction
  No Ozone Reaction Estimation

Fraction sorbed to airborne particulates (phi)
0.00144 (Junge, Mackay)
0.000151 (Koa Method)

Note The sorbed fraction may be resistant to atmospheric oxidation

11. Soil Adsorption Coefficient (PCKOCWIN v1.66)

	MCI Method	Kow Method
Koc	284.4	307.8

Log Koc	2.454	2.488

12. Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1.67]

Rate constants can NOT be estimated for this structure!

13. Bioaccumulation Estimates from Log Kow (BCFWIN v2.17)

Log BCF from regression-based method = 2.019 (BCF = 104.5 L/kg wet-wt)
Log Biotransformation Half-life (HL) = 0.3185 (HL = 2.082 days)
Log BCF Arnot-Gobas method (upper trophic) = 2.430 (BCF = 268.9)
Log BAF Arnot-Gobas method (upper trophic) = 2.430 (BAF = 269.1)
Log Kow used = 3.57 (estimated)

14. Volatilization from Water

Henry LC = 3.15E-006 atm-m^3/mole (estimated by Group SAR Method)
Half-Life from Model River = 252.3 hours (10.51 days)
Half-Life from Model Lake = 2866 hours (119.4 days)

15. Removal In Wastewater Treatment

Total removal = 14.87 %
Total biodegradation = 0.20 %
Total sludge adsorption =14.52 %
Total to Air = 0.15 %
(Using 10000 hr Bio P, A, S)

16. Level III Fugacity Model

	Mass Amount (%)	Half-Life (hr)	Emissions (kg/hr)
Air	0.484	11.5	1000
Water	20.2	900	1000
Soil	78.9	1.8E003	1000
Sediment	0.326	8.1E003	0

Persistence Time 1.07e+003 hr.

VITA

Kumar Sharad Samant

Candidate for the Degree of

Master of Science

Thesis CORRELATING MOLECULAR STRUCTURES AND PROPERTIES OF EMERGING CONTAMINANTS WITH ENVIRONMENTAL FATE MODELS

Major Field: Environmental Engineering

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Country of Citizenship India

Education

Completed the requirements for the Master of Science in Environmental Engineering at Oklahoma State University, Stillwater, Oklahoma in May, 2010.

Completed the requirements for the Bachelor of Science/Arts in Civil Engineering at University of Mumbai, Mumbai, Maharashtra/India in 2007.

Experience

Junior Site Engineer in Kalpataru Properties Pvt. Ltd., Mumbai, India.
Teaching Assistant at Oklahoma State University, Stillwater, Oklahoma.

Professional Memberships
Chi Epsilon.

Name Kumar Sharad Samant Date of Degree May, 2010

Institution Oklahoma State University Location Stillwater, Oklahoma

Title of Study CORRELATING MOLECULAR STRUCTURES AND PROPERTIES OF EMERGING CONTAMINANTS WITH ENVIRONMENTAL FATE MODELS

Pages in Study 166 Candidate for the Degree of Master of Science

Major Field Environmental Engineering

Scope and Method of Study

The purpose of this work is to perform a preliminary analysis for future use in a full-scale quantitative structure-activity relationship (QSAR) analysis to ultimately predict the biodegradation, oxidation and hydrolysis rates of emerging chemicals of environmental concern. Computational chemistry software like Estimation Program Interface suite and Molecular Modeling Pro program were used to calculate physicochemical properties. Simple linear regression method was used for statistical analysis of the data.

Findings and Conclusions

A preliminary analysis of quantitative structure-activity relationships was conducted over six selected compounds geosmin, 2-methylisoborneol, 2,4-dichlorophenol, acetaminophen, triclosan and atrazine. Multiple structural, thermodynamic, atomic, electronic and energy descriptors were examined in regards to their correlations with biodegradation, oxidation and hydrolysis rate constants Statistical analysis of the data suggested there are various potential descriptors to predict the activity of these chemicals. Most notably, the descriptors log octanol-air partition coefficient, E_{HOMO}, E_{LUMO} displayed the highest correlations for the biodegradation rate constant, oxidation rate constant and hydrolysis rate constant respectively. Future areas of research might include additional compounds to examine compilation of data for a particular measurement from references originating within the same laboratory and measurement system and investigate other techniques to build QSARs models.

ADVISER'S APPROVAL Dr. John Veenstra