Solvents Exercise

One of the primary goals of the solvents lecture is to give the participants an understanding of how the physicochemical and hazardous properties of solvents effect safety and environmental impact. For example, the property of vapor pressure is directly related to emissions of volatile organic compounds (VOCs) and therefore is relevant to worker health and safety, and to clean air in communities. This activity should be used after various solvent properties are explained in order to show how the connection between properties and effects is made in real-world situations.

This activity uses published solvent selection guides generated by a major pharmaceutical company, which uses them to evaluate solvents used in their large-scale process chemistry. The company has rated each solvent according to nine criteria on a "red-yellow-green"/traffic light scale, based on the physicochemical and hazardous properties (which are also summarized).

Participants should be divided into groups of 4-5 and provided with the solvent cards for acetic acid and cyclohexene, with the names of the solvents and the "red-yellow-green" ratings left blank. The groups should be given approximately 20 minutes to discuss the chemical data provided on the cards and provide their own ratings in each of the nine categories. The solvent identities are left blank to avoid biasing the evaluation (i.e., the word "acid" has negative connotations that may confuse non-chemists).

The debriefing will also take approximately 20 minutes. The groups will be asked to report which criteria received a green light and which criteria received a red light and the results will then be tabulated. Then the solvent identities and actual red-yellow-green ratings from the pharmaceutical industry scientists should be revealed. This is likely to result in some "what were they thinking?" comments from the participants. This should lead to a discussion which should focus on the following issues:

1. How much the ratings change depending on the way the solvent is used in industry (i.e., compare a situation where a worker is cleaning the inside of a tank with a situation where solvent is part of an effluent that is being released into a river). The answer - a lot.
2. Is it possible that either of these solvents will ever receive all "green lights" in every category? The answer - almost certainly not. This can function as a segue into a discussion of alternative solvents being developed by green chemists.

This activity requires participants to convert the “dry” numbers seen in the list of solvent property data into a framework that can be used to make decisions that are faced in the real world. It highlights the ambiguities that can arise from this kind of process but at the same time reinforces the connection between chemical structure, properties, and the larger-scale consequences. This should provide some food for thought as the lecture transitions into “green solvents” and is related to the overall course themes related to designing safer chemicals.

The solvent cards and the answers are provided below.

Solvent 1

Incineration
Recycle
Biotreatability
VOC emission
Environmental impact to water
Environmental impact to air
Health hazard
Exposure potential
Safety hazard

major issues have been identified; appropriate control procedures need to be in place.

issues have been identified; the need for control procedures should be considered.

no major issues have been identified in this area.

ICH category	3	Permitted daily exposure limit (mg/day)	> 50

Molecular wt	60.05
Melting point (°C)	17
Boiling point (°C)	118
Vapor pressure (mm)	15.5
Solubility in water (gm/L)	Miscible.
Odor threshold (ppm)	0.1 - 0.2
Density	1.05
Vapor density (air = 1)	2.07
Log K_{ow}	-0.17
Worst case ecotoxicity EC_{50} (mg/L) [species]	47 [daphnia]
Degradation in water	Biodegradable.
Ozone creation potential POCP	16
Half life for evaporation from a river (days)	Very slow
Exposure limit [ACGIH 8hr TWA] (ppm)	10
Flash point (°C)	39
Conductivity (Ps/M)	1120000
Risk phrase(s)	Flammable. Causes severe burns.
Heat of combustion (Btu/lb)	5645
Dielectric constant	6.2
Autoignition temperature (°C)	426

AZEOTROPE DATA

The following azeotropes (excluding zeotropes) with other solvents have been reported:

Solvent	%solvent 1	bp (°C)
Cyclohexane	9.6	78.8
Dioxane	77	119.5
Ethyl benzene	66	114.6
Heptane	33	91.7
Hexane	6	68.5
Nitroethane	30	112.4
Pyridine	51	138.1
Toluene	28	100.6
Triethylamine	67	163
Xylene	72	115.3

Solvent 2

Incineration
Recycle
Biotreatability
VOC emission
Environmental impact to water
Environmental impact to air
Health hazard
Exposure potential
Safety hazard

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ICH category	2	Permitted daily exposure limit (mg/day)	38.8

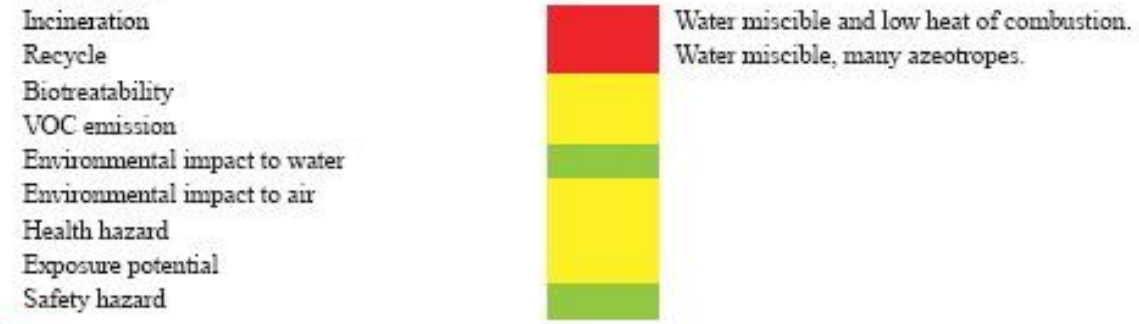
Molecular wt	84.2
Melting point (°C)	7
Boiling point (°C)	81
Vapor pressure (mm)	98
Solubility in water (gm/L)	0.06
Odor threshold (ppm)	300
Density	0.78
Vapor density (air= 1)	2.9
Log K_{ow}	3.44
Worst case ecotoxicity EC_{50} (mg/L) [species]	3.8 [algae]
Degradation in water	Slow biodegradation.
Ozone creation potential POCP	60
Half life for evaporation from a river (days)	0.15
Exposure limit [ACGIH 8hr TWA] (ppm)	300
Flash point (°C)	-20
Conductivity (Ps/M)	2
Risk phrase	Highly flammable.
Heat of combustion (Btu/lb)	18684
Dielectric constant	2.02
Autoignition temperature (°C)	245

AZEOTROPE DATA

The following azeotropes (excluding zeotropes) with other common solvents have been reported:

Solvent	% solvent 2	bp (°C)
Acetic acid	91.4	78.8
Methyl ethyl ketone	60	71.8
Methyl acetate	22	55.5
Methanol	63.6	53.9
Isopropanol	68	69.4
Ethyl acetate	44	71.6
Acetone	32.5	53
1-Butanol	90 – 95	80 - 82

Acetic acid



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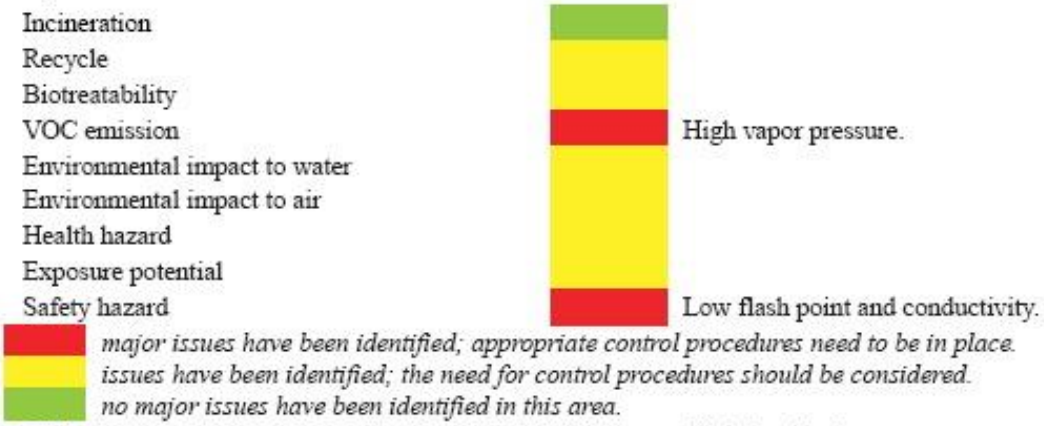
Cyclohexane



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