

Getting Started

Follow the steps below for a "guided tour" of the CRW. You'll create a mixture of chemicals, analyze the potential reactivity hazards from mixing those chemicals, and work with other key features of the CRW.

Creating a new mixture of chemicals

You're new on the staff of a small specialty chemical company, and have been assigned to be assistant manager of the main chemical storage warehouse. You need to be sure that all chemicals in the warehouse are stored as safely as possible.

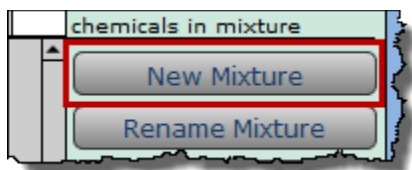
You do a walk-through of the warehouse, and note that the following four chemicals are stored on the same pallet within the warehouse:

- Diethyl ether
- Acetyl chloride
- Benzene
- Sodium hydroxide (solid)

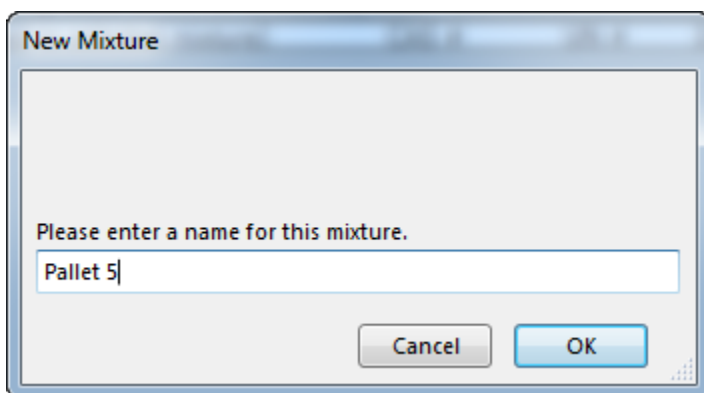
You need to know the reactivity hazards if they were to accidentally mix. You also need to check whether any should be moved to a different storage location.

Follow the steps below to assess the hazards:

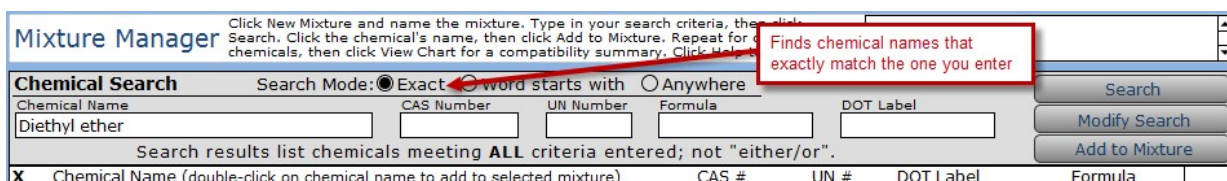
1. You first must create a new mixture, to which you'll add the four chemicals on the pallet. If you're not viewing the Mixture Manager screen, click Mixture Manager in the taskbar at the top of the CRW screen. You use this taskbar to navigate among all the main CRW screens.
2. Click New Mixture (in the lower left corner of the Mixture Manager).



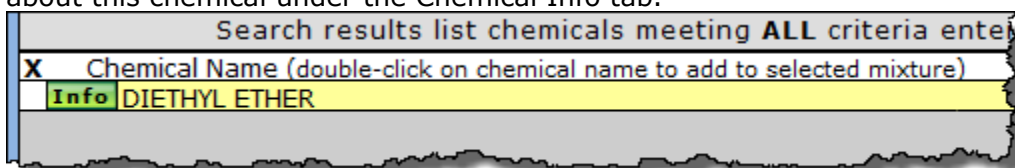
3. Type a name for the mixture, such as "Pallet 5", and then click OK. The new mixture is created. It represents the storage pallet. Next, you'll add the four chemicals to it, starting with Diethyl ether.



4. Type "Diethyl ether" in the Chemical Name box, click the "Exact" button, and then click Search. An Exact search finds only those chemicals with names (or name synonyms) spelled exactly like the name you type. The record for diethyl ether is found in this search.



5. Click the green 'Info' button immediately to the left of the name, DIETHYL ETHER. The chemical datasheet for diethyl ether displays. The datasheet contains basic information about this chemical under the Chemical Info tab.



6. Note the Reactive Group(s) list. A reactive group is a category of chemicals that react in a characteristic way. Diethyl ether is assigned to the "Ethers" reactive group. To predict potential reactivity between any pair of chemicals, the CRW first identifies the assigned reactive group(s) for each of the chemicals, then predicts the kind of reactions likely to occur if members of these groups are mixed together.

Next, click the Physical Properties and Synonyms tabs to review diethyl ether's physical properties and name synonyms.

Chemical Datasheet for: **DIETHYL ETHER**
Included in 1 mixture

[Mixture Manager](#) | [Mixture Report](#) | [Compatibility Chart](#) | [Reactive Groups](#) | [Custom Chemicals](#) | [Absorbent Incompatibilities](#) | [Materials of Construction](#) | [Data Sharing](#) | [Help](#)

[Chemical Info](#) | [Physical Properties](#) | [Synonyms](#)

CAS Number	UN/NA Number	USCG CHRIS Code	Chemical Formula
60-29-7	1155	EET	C4H10O

DOT Hazard Label: Flammable Liquid
Reactive Group(s): Ethers
Reactivity Alert(s): Highly Flammable; Peroxidizable Compound

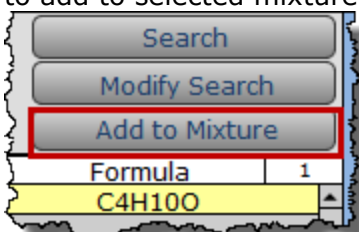
General Description: A clear colorless liquid with an anesthetic odor. Flash point -49°F. Less dense than water and slightly soluble in water. Hence floats on water. Vapors are heavier than air. Used as a solvent and to make other chemicals.

Reactivity Profile: Occasional explosions have occurred when aluminum hydride was stored in ether. The explosions have been blamed on the presence of carbon dioxide impurity in the ether, [J. Amer. Chem. Soc. 70:877 (1948)]. Diethyl ether and chromium trioxide react violently at room temperature. Solid acetyl peroxide in contact with ether or any volatile solvent may explode violently. A 5-gram portion in ether detonated while being carried, [Chem. Eng. News 27:175(1949)]. Nitrosyl perchlorate ignites and explodes with diethyl ether. A mixture of ether and ozone forms aldehyde and acetic acid and a heavy liquid, ethyl peroxide, an explosive, [Mellor 1:911(1946 -1947)].

Air and Water Reactions	Health Hazards	Potentially Incompatible Absorbents
Highly flammable. Oxidizes readily in air to form unstable peroxides that may explode spontaneously [Bretherick, 1979 p.151 -154, 164]. A mixture of liquid air and diethyl ether exploded spontaneously, [MCA Case History 616(1960)].	Vapor inhalation may cause headache, nausea, vomiting, and loss of consciousness. Contact with eyes will be irritating. Skin contact from clothing wet with the chemical may cause burns. (USCG, 1999)	

NFPA Flammability 1, Instability 1, Health Special 4

- Click Mixture Manager in the taskbar to redisplay the Mixture Manager.
- Click Add to Mixture to add Diethyl Ether to the mixture or double-click on chemical name to add to selected mixture



Its name is added to the mixture list:

Mixture: Palet 5		3 mixtures available	
Chemical / Reactive Group Name	CAS Number	RG Number(s)	1
Info DIETHYL ETHER	60-29-7	14	

- To try another of the three available search modes, click Word starts with, type "acetyl" into the Chemical Name box, and then click Search. This search finds all chemicals with names (or name synonyms) beginning with "acetyl."

Chemical Search Search Mode: Exact Word starts with Anywhere

Chemical Name: CAS Number: UN Number: Formula: DOT Label:

Search results list chemicals meeting **ALL** criteria entered

Chemical Name (double-click on chemical name to add to selected mixture)

Finds chemical names that start with the characters you enter

Buttons: Search, Modify Search, Add to Mixture

10. Scroll down the list of found chemicals to find Acetyl chloride. Click to select it, then click Add to Mixture. This chemical is added to the list of chemicals in your mixture.
11. To try out the remaining search mode, type "Benzene" in the Chemical Name box, click the "Anywhere" button, then click Search.

Chemical Search Search Mode: Exact Word starts with Anywhere

Chemical Name: CAS Number: UN Number: Formula: DOT Label:

Search results list chemicals meeting **ALL** criteria entered; not "either/or".

Chemical Name (double-click on chemical name to add to selected mixture)

Finds chemicals with names containing the character string you enter

Buttons: Search, Modify Search, Add to Mixture

A long list of matching chemicals displays. Each contains "benzene" somewhere in its name or name synonym, including benzene (located about a third of the way down from the top of the list).

12. To narrow this search, click Modify Search to redisplay "benzene" in the Chemical Name field, click Exact, and then click Search. This time, only benzene is found.
13. Double-click on Benzene to add it to the mixture. It is added to the list of chemicals in your mixture.
14. To add the last of the four chemicals to your mixture, type Sodium hydroxide in the Chemical Name box, leave Exact selected, then click Search. Click "Sodium hydroxide, solid" to select it, then click Add to Mixture. Your mixture now contains four chemicals:

Mixture: Palet 5		3 mixtures available	
Chemical / Reactive Group Name	CAS Number	RG Number(s)	
Info ACETYL CHLORIDE	75-36-5	40	4
Info BENZENE	71-43-2	16	
Info DIETHYL ETHER	60-29-7	14	
Info SODIUM HYDROXIDE, SOLID	1310-73-2	10	

Evaluating overall reactivity hazards

Now that you've added the four chemicals, you need to evaluate their reactivity hazards and determine whether any should be moved from the pallet to a different storage location.

1. Click View Chart in the lower right corner of the Mixture Manager screen (or click Compatibility Chart in the taskbar). The Compatibility Chart displays. The color-coded cells in the chart represent compatibility predictions for all possible pairs of chemicals in the mixture. That is, each cell represents the potential reactivity (if any) from mixing two of the chemicals together. To find out how any pair of chemicals in the mixture could react, you find the intersecting cell.
2. To find out how benzene and acetyl chloride could react, based on known reactivity between the reactive groups to which they belong, find the intersecting cell. This cell is color-coded yellow and displays a "C" to indicate that mixing these two chemicals could be hazardous under certain conditions. Look in the chart legend below the chart to see the definition for each of the color and letter codes used in the chart.

If a pair of chemicals are incompatible (a reaction is possible), the intersecting cell is red, with "N" (representing "no, not compatible; hazardous reactivity issues are expected") displayed within it.

If mixing the pair of chemicals could be hazardous under certain conditions, the intersecting cell is yellow, with "C" (representing "caution, may be hazardous under certain conditions") displayed within it.

If the chemicals are compatible (no reaction is predicted), the intersecting cell is green with "Y" (representing "yes, compatible; no hazardous reactivity issues expected") displayed within it.

- To learn more about potential reactivity between benzene and acetyl chloride, click the intersecting cell. A summary of potential reactivity between these two chemicals displays below the chart, under the Hazard Summary tab. You can see that heat and gases would be released if these chemicals react. To the right of the hazard summary, the intrinsic hazards of each of the four chemicals are listed. Further to the right is the chart legend.

The screenshot displays the software interface with a compatibility chart and a hazard summary. The compatibility chart shows the following data:

Health	Flammability	Instability	Special	ACETYL CHLORIDE	BENZENE	DIETHYL ETHER	SODIUM HYDROXIDE, SOLID
3	3	2	2	ACETYL CHLORIDE			
2	3	0		BENZENE	C		
1	4	1		DIETHYL ETHER	N	Y	
3	0	1		SODIUM HYDROXIDE, SOLID	N	Y	Y

The Hazard Summary tab is selected, showing the following information:

Selected Chemical Combination: BENZENE, ACETYL CHLORIDE

Reaction products may be corrosive
Reaction liberates gaseous products and may cause pressurization
Exothermic reaction at ambient temperatures (releases heat)

Chemical Intrinsic Hazards:

- ACETYL CHLORIDE: Highly Flammable; Water-Reactive; Air-Reactive
- BENZENE: Highly Flammable
- DIETHYL ETHER: Highly Flammable; Peroxidizable Compound
- SODIUM HYDROXIDE, SOLID: Water-Reactive

Chart Legend:

- Y: Compatible** - No hazardous reactivity issues expected.
- N: Incompatible** - Hazardous reactivity issues are expected.
- C: Caution** - May be hazardous under certain conditions.
- SR: Self-Reactive** - Potentially Self-Reactive (e.g., polymerizable)

***Note:** If asterisk appears in cell, then compatibility decision was manually changed by the user from the CRW prediction to that shown.

- Click the Potential Gases tab to learn which gas byproducts would be generated if benzene and acetyl chloride were to react. Hydrogen halide gases could be generated in the reaction.

The screenshot displays the software interface with the Potential Gases tab selected. The following information is shown:

Selected Chemical Combination: BENZENE, ACETYL CHLORIDE

Potential Gases: Hydrogen Halide

- Click the Documentation tab. Under this tab is background documentation summarizing the reasons behind the predictions, including reference source citations when possible.

Background documentation is based on reactivity between the reactive groups to which the chemicals belong: in this case benzene is in the Aromatic Hydrocarbons reactive group, and acetyl chloride is in the Acid halides, Sulfonyl Halides, and Chloroformates reactive group.

Hazard Summary	Potential Gases	Documentation	Mixture Comments
Selected Chemical Combination	BENZENE ACETYL CHLORIDE		
<p>Hydrocarbons, Aromatic WITH Acyl Halides, Sulfonyl Halides, and Chloroformates:</p> <p>Benzene may liberate toxic HX gases upon reaction with the respective diatomic halogens or through reaction with the corresponding acyl halides (Rodd, E. H, Ed. Chemistry of Organic Compounds. New York: Elsevier Publishing Company, 1951. Vol. III pp. 90, 96-97).</p> <p>The Friedel-Crafts acylation reaction between acyl halides and aromatic hydrocarbons generates HX gas and an aromatic ketone. However, this reaction requires a Lewis acid catalyst such as AlCl₃ and will not occur on its own (Loudon, Marc. 2002. Organic Chemistry. 4th ed. New York: Oxford University Press. p. 713).</p>			

- Click the Mixture Comments tab. Under this tab, you can add your own comments and references related to the mixture representing all the chemicals on the pallet. Your comments are automatically saved unless you delete them.
- Review the Chemical Intrinsic Hazards field, which lists the intrinsic hazards of each chemical represented in the chart.
- Scroll the chart further to the right, as needed, to review the Chart Legend. Here, you can find the definition for each kind of color-coded cell you may see in a Compatibility Chart.
- Click additional chart cells to observe predicted reactivity and documentation for other pairs of chemicals.
- Click Chemical Pairs. The Chemical Pair Analysis screen displays. If you need to work with a compatibility chart for a mixture of many chemicals (you can include up to 100 chemicals in any mixture), it can be hard to find and click the chart cell representing a particular pair of chemicals. In such a situation, the Chemical Pairs button makes it much easier to select and view reactivity predictions for a particular pair of chemicals in the chart.

Print Chart

Export Chart Data

NFPA

Health Flammability Instability Special

3 3 2 No

2 3 0

ACETYL CHLORIDE

BENZENE

C

Chemical Pairs

Pallet 5 Compatibility Chart

- Select any two of the chemicals in the mixture, review the compatibility predictions for this pair of chemicals, and then click the close box in the upper right corner of the window.

Chemical Pair Analysis

Select the chemicals to be compared from the current mixture

1 - Chemical or Reactive Group
ACETYL CHLORIDE

2 - Chemical or Reactive Group
BENZENE

View this chemical's datasheet

Flammability

Health 3 3 2 Reactivity

Special

View this chemical's datasheet

Flammability

Health 2 3 0 Reactivity

Special

Selected chemicals compatibility **C**

Control-click to override default rating.
Shift-click to reset to default (original) rating.

Hazard Summary Potential Gases Documentation Pair Comments

Reaction products may be corrosive
Reaction liberates gaseous products and may cause pressurization
Exothermic reaction at ambient temperatures (releases heat)

Removing a chemical from the mixture

As the warehouse manager, you might choose to move a chemical from the pallet if there is a high likelihood of a reaction between it and any other chemicals on the pallet. Pairs of chemicals that are very likely to react with each other are represented by the red cells on the chart.

1. Check for red and yellow cells in the chart to determine which chemical(s) are predicted to be incompatible with which other chemicals on the pallet. Red cells represent chemical pairs that are generally incompatible. Yellow cells represent pairs that are incompatible under certain conditions.
2. Note that all cells representing the mixture of acetyl chloride with other chemicals are either red or yellow, indicating that acetyl chloride is incompatible with all the other chemicals on the pallet (at least under some conditions, in the case of benzene). The green color-coding of all other possible chemical pairs indicates that the other three chemicals are predicted to be compatible with each other. As the warehouse assistant manager, you decide to remove the acetyl chloride from the pallet.

As the acetyl chloride is moved to another storage location, you also remove it from the mixture representing the chemicals on the pallet:

1. Click Mixture Manager in the taskbar. The Mixture Manager displays.

- Click the square red button to the right of "ACETYL CHLORIDE" in the list of chemicals in the mixture, then click OK. This chemical is removed from the mixture (but is *not* removed from the CRW's chemical database).

Mixture: Pallet 5		4 mixtures available	
Chemical / Reactive Group Name	CAS Number	RG Number(s)	
Info ACETYL CHLORIDE	75-36-5	40	
Info BENZENE	71-43-2	16	
Info DIETHYL ETHER	60-29-7	14	
Info SODIUM HYDROXIDE, SOLID	1310-73-2	10	

- Click View Chart (or Compatibility Chart in the taskbar). The green cells in the chart indicate that no incompatibilities are predicted among the remaining three chemicals stored on the pallet.

Print Chart		Export Chart Data		NFPA		Chemical Pairs	
Health	Flammability	Instability	Special	Pallet 5 Compatibility Chart			
				BENZENE	DIETHYL ETHER	SODIUM HYDROXIDE, SOLID	
2	3	0					
1	4	1		Y			
3	0	1		Y	Y		

Evaluating water reactivity

You learn that a major storm is coming, bringing a possibility of flooding in your warehouse. You want to determine the potential reactivity hazards if the chemicals on the pallet were to come into contact with water.

To do that, you'll add water to your mixture of chemicals:

- Click Mixture Manager in the taskbar.
- Add water to the mixture by clicking on the drop-down list under "Add:" in the lower-right corner of the Mixture Manager screen and selecting Water. Water is added to the mixture of chemicals. (TIP: Alternatively, you could have added water to the mixture by searching for the chemical name, "water.")

Mixture: **Pallet 5** 5 mixtures available Selected mixture last modified: 12/29/2015 3:07:56 PM

Chemical / Reactive Group Name	CAS Number	RG Number(s)	chemicals in mixture
Info ACETYL CHLORIDE	75-36-5	40	
Info BENZENE	71-43-2	16	
Info DIETHYL ETHER	60-29-7	14	
Info SODIUM HYDROXIDE, SOLID	1310-73-2	10	

Buttons: New Mixture, View Chart

Reactive Group Selection: Air, Nitrogen, Water (highlighted), Reactive Group

3. Click View Chart (or Compatibility Chart in the taskbar). The compatibility chart displays. Cell color-coding indicates that benzene and diethyl ether are compatible with water (green-coded cells), but sodium hydroxide is not (yellow-coded cell). Depending on the likelihood of water entering your warehouse and contacting the chemicals on the pallet, you should consider protecting the sodium hydroxide from contact with water. For the purposes of this guided tour, leave the sodium hydroxide in the mixture.

Print Chart
Export Chart Data
NFPA Chemical Pairs

Health
Flammability
Instability
Special

Pallet 5
Compatibility
Chart

				BENZENE	DIETHYL ETHER	SODIUM HYDROXIDE, SOLID	WATER
2	3	0					
1	4	1		Y			
3	0	1		Y	Y		
				Y	Y	C	

Working with a reactive group

The storm has passed, and no water entered your warehouse. If you'd like, you can remove water from your mixture, just as you removed acetyl chloride.

Now the warehouse manager has added another container to the pallet, and has left on an adventure travel trip to a remote location. The container label is water damaged, so you can read only part of the name: "acrylate." While the manager is away, you want to update the information about the materials on the pallet to include this new chemical, as best you can, and verify that it can be safely stored with the other chemicals now on the pallet.

You could try a search for chemicals that have "acrylate" anywhere in their names, but that search would find dozens of chemicals (go ahead and try it!). Since you are not sure which chemical it is, your better bet is to add the chemical's reactive group to your mixture. You know that it is an acrylate, and therefore would belong to the "Acrylates and Acrylic Acids" reactive group.

1. Click Mixture Manager in the taskbar, then click on the "Add:" drop-down menu in the lower-right corner of the screen and select "Reactive Group". The Reactive Group Information screen displays. (Tip: Another way to display this screen is to click Reactive Groups in the taskbar.)
2. In the list of all reactive groups, click on the "Acrylates and Acrylic Acids" reactive group. A description of this reactive group displays. Review the description.
3. Click Add Selected Group to Mixture. Click Yes to indicate that you want to add this group to your mixture representing the chemicals on the pallet.

Reactive Group Information

Add Selected Group to Mixture

1. Reactive Group Category

All

Click once on reactive group name to select

	RG #
Acetals, Ketals, Hemiacetals, and Hemiketals	70
Acids, Carboxylic	3
Acids, Strong Non-oxidizing	1
Acids, Strong Oxidizing	2
Acids, Weak	60
Acrylates and Acrylic Acids	71
Acyl Halides, Sulfonyl Halides, and Chloroformates	40
Alcohols and Polyols	4
Aldehydes	5
Alkynes, with Acetylenic Hydrogen	63
Alkynes, with No Acetylenic Hydrogen	64
Amides and Imides	6
Amines, Aromatic	68
Amines, Phosphines, and Pyridines	7
Anhydrides	37
Aryl Halides	66
Azo, Diazo, Azido, Hydrazine, and Azide Compounds	8
Bases, Strong	10
Bases, Weak	61
Carbamates	9
Carbonate Salts	62
Chlorosilanes	55
Conjugated Dienes	65
Cyanides, Inorganic	11
Diazonium Salts	25
Epoxides	34
Esters, Sulfate Esters, Phosphate Esters, Thiophosphate Esters, and Borate	13
Ethers	14
Fluoride Salts, Soluble	48
Fluorinated Organic Compounds	47
Halogenated Organic Compounds	17

Description of: Acrylates and Acrylic Acids

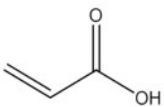
FLAMMABILITY - Many of the acrylate esters, e.g. methyl methacrylate, have relatively high vapor pressures and are highly flammable, with flash points below 100 deg C.

REACTIVITY - Acrylic acid and its esters readily combine with themselves (to form polyacrylic acid) or other monomers (e.g. acrylamides, acrylonitrile, vinyl, styrene, and butadiene) by reacting at their double bond, forming homopolymers or copolymers.

These materials are capable of thermally induced or chemically initiated radical type polymerization reactions which can generate significant amounts of heat (up to -100 kJ/mol). This can result in large adiabatic temperature rises, which also can trigger gassy decomposition reactions.

These materials are typically inhibited with low levels (ppm range) of antioxidants to prevent premature polymerization chain reactions and these inhibitors may require dissolved oxygen to be effective. The inhibitors can be depleted with time and are depleted faster at higher storage temperatures. These materials are known to be susceptible to destabilization due to contaminants, even at low levels of contamination. Although there are obvious contaminants

Structural Formula Example(s) for: Acrylates and Acrylic Acids



Acrylic acid

The Mixture Manager displays, and "Acrylates, Acrylic Acids" is added to the list of chemicals in your mixture.

4. Click View Chart. The compatibility chart displays. Now it contains a red cell representing the reaction between the sodium hydroxide and the "Acrylates and Acrylic Acids" reactive group. There are also two new yellow cells representing the reaction of the "Acrylates and Acrylic Acids" reactive group with benzene and diethyl ether. (If you left water in your mixture, there's now also a new yellow cell representing the reaction between water and the "Acrylates and Acrylic Acids" reactive group.) Click the red cell representing the reaction between sodium hydroxide and the "Acrylates and Acrylic Acids" reactive group, then review the Hazard Summary discussion. Note the potential for an explosive reaction if these two substances were to mix. Click the Potential Gases and Documentation tabs to review further details about the potential reactivity between this pair of chemicals. The documentation alerts you that acrylates are polymerizable, and often are inhibited with antioxidants. Inhibitor depletion may be a concern for this chemical.
5. On the Compatibility Chart, cells on the diagonal represent the mixture of a chemical with itself. Most cells on the diagonal are grey and display no letter code, indicating that no self-

reactivity is expected. Notice, though, that the cell representing the mixture of an acrylate or acrylic acid with itself is yellow and displays a "SR" letter code. Refer to the Chart Legend to see that the yellow color and "SR" code indicates that the chemical is potentially self-reactive.

It would be a reasonable management decision to remove the acrylate from the pallet, and to monitor it for signs of polymerization.

This concludes your guided tour of the Chemical Reactivity Worksheet. To delete the mixture you created, return to the Mixture Manager, check that the mixture is selected in the Mixture drop-down list, then click Delete Mixture. Check other Help topics to learn more about the CRW.