



Encoding Reactive Chemical Hazards and Incompatibilities in an Alerting System

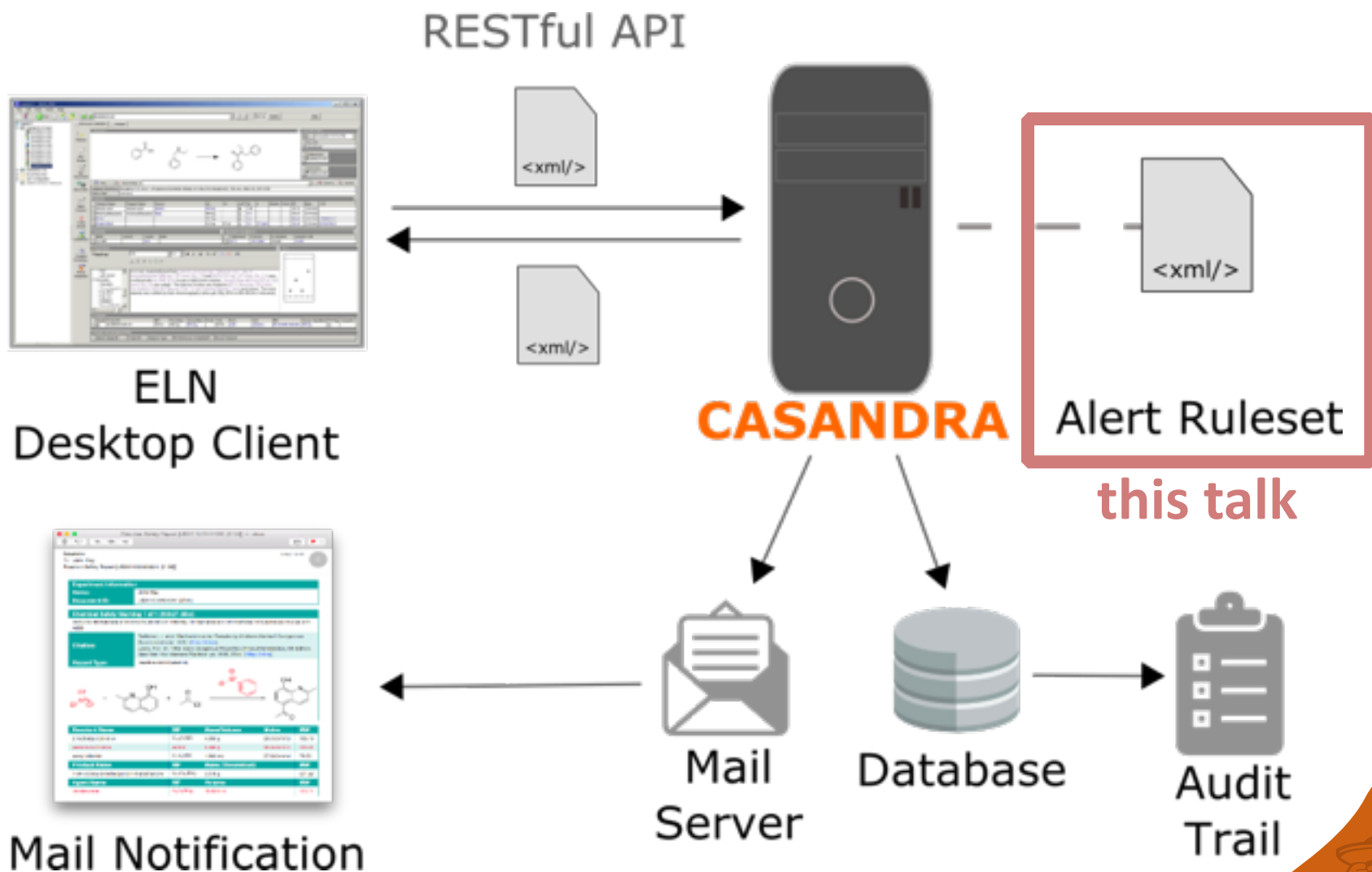
John May and Roger Sayle

NextMove Software

Cambridge, UK



MOTIVATION (THE ALERTING SYSTEM)



Casandra

Today 14:23

To: John May

Reaction Safety Report [US20110224242A1 [0108]]

Experiment Information

Name: John May
 Document ID: US20110224242A1 [0108]

Chemical Safety Warning 1 of 1 [RG:27-38:c]

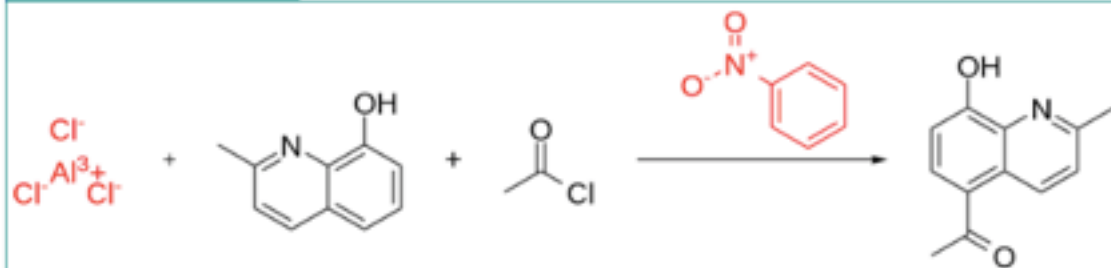
Contains nitrobenzene and contains aluminium chloride, nitrobenzene and nitromethane form explosive mixtures with AlCl₃

Citation:

Reithman, J. et al. Mechanismus der Zersetzung nitrobenzoler Lösungen von Aluminiumchlorid. 1976. ([Wiley Online](#))
 Lewis, R.J., Sr. 1992. Sax's Dangerous Properties of Industrial Materials, 8th Edition. New York: Van Nostrand Reinhold. pp. 2518, 2544. ([Wiley Online](#))

Hazard Type:

Reactive Incompatibility



Reactant Name	MF	Mass/Volume	Moles	MW
2-methylquinolin-8-ol	C ₁₀ H ₉ NO	4.000 g	25.130 mmol	159.18
aluminium chloride	Al ₂ Cl ₆	8.380 g	62.820 mmol	133.34
acetyl chloride	C ₂ H ₃ ClO	1.960 mL	27.640 mmol	78.50
Product Name	MF	Mass (Theoretical)		MW
1-(8-hydroxy-2-methylquinolin-5-yl)ethanone	C ₁₂ H ₁₁ NO ₂	3.510 g		201.22
Agent Name	MF	Volume		MW
nitrobenzene	C ₆ H ₅ NO ₂	10.000 mL		123.11

Reason,
 Primary Citations,
 Category

EVOLUTION OF HAZARD ALERTING

1. Chemical Compound (MSDS) Lookup
 - a. Exact name/MFCD/Synonym comparison
 - b. Name-to-structure canonical match
 - c. Normalised representation (InChI) match
2. Chemical Incompatibility Lookup
3. Substructure Patterns
4. Chemical Class Incompatibility
5. Reaction Mechanism Recognition (+ H₂ Gas)
6. Physical Property Thresholds (BP, HoD, VP)

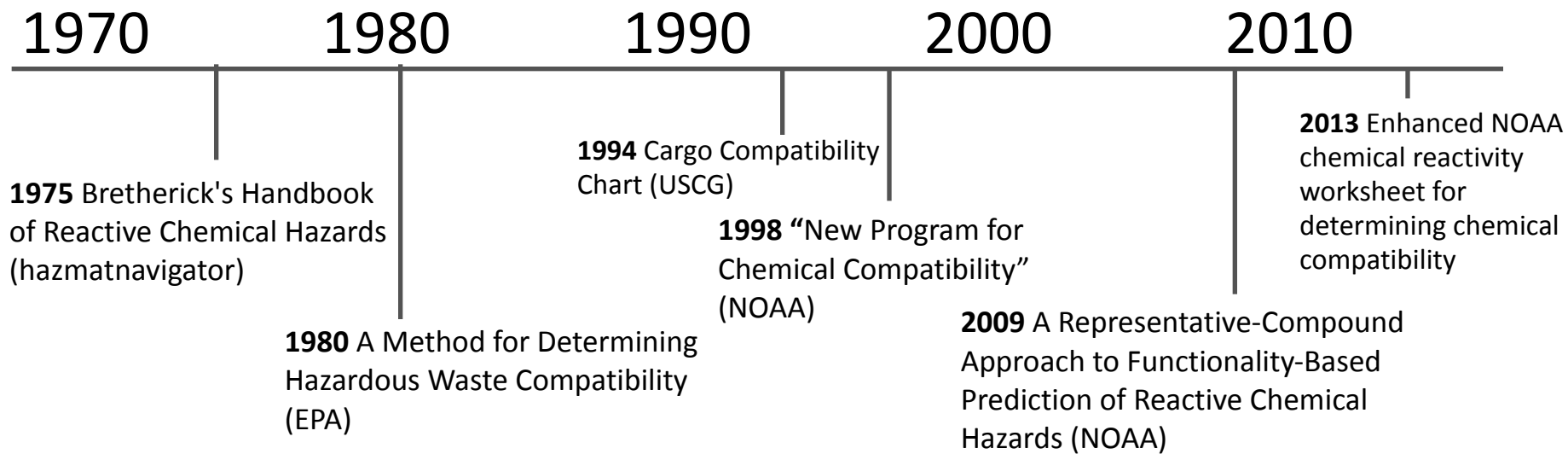
Known
Knowns

Known
Unknowns



HAZARD COMPATABILITY TIMELINE

(INCOMPLETE)



REACTIVE GROUPS

REACTIVE GROUPS

CARGO GROUPS

	1. NON-OXIDIZING MINERAL ACIDS	2. SULFURIC ACID	3. NITRIC ACID	4. ORGANIC ACIDS	5. CAUSTICS	6. AMMONIA	7. ALIPHATIC AMINES	8. ALKANOLAMINES	9. AROMATIC AMINES	10. AMIDES	11. ORGANIC ANHYDRIDES	12. ISOCYANATES	13. VINYL ACETATE	14. ACRYLATES	15. SUBSTITUTED ALLYLS	16. ALKYLENE OXIDES	17. EPICHLOROHYDRIN	18. KETONES	19. ALDEHYDES	20. ALCOHOLS, GLYCOLS	21. PHENOLS, CRESOLS	22. CAPROLACTAM SOLUTION			
1. NON-OXIDIZING MINERAL ACIDS		X																						1	
2. SULFURIC ACID	X		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X		2
3. NITRIC ACID		X																							3
4. ORGANIC ACIDS		X																							4
5. CAUSTICS	X	X	X	X							X	X				X	X			X	X	X	X		5
6. AMMONIA	X	X	X	X						X	X	X	X			X	X			X	X	X	X		6
7. ALIPHATIC AMINES	X	X	X	X							X	X	X	X	X	X	X	X	X	X	X	X	X		7
8. ALKANOLAMINES	X	X	X	X							X	X	X	X	X	X	X			X	X	X	X		8
9. AROMATIC AMINES	X	X	X								X	X								X					9
10. AMIDES	X	X	X			X																X			10
11. ORGANIC ANHYDRIDES	X	X	X		X	X	X	X	X																11
12. ISOCYANATES	X	X	X	X	X	X	X	X	X	X												X	X		12
13. VINYL ACETATE	X	X	X			X	X	X																	13
14. ACRYLATES			X	X			X	X																	14
15. SUBSTITUTED ALLYLS			X	X			X	X																	15
16. ALKYLENE OXIDES	X	X	X	X	X	X	X	X																	16
17. EPICHLOROHYDRIN	X	X	X	X	X	X	X	X																	17
18. KETONES		X	X			X																			18
19. ALDEHYDES		X	X		X	X	X	X	X																19
20. ALCOHOLS, GLYCOLS		X	X		X	X						X													20
21. PHENOLS, CRESOLS		X	X		X	X				X															21
22. CAPROLACTAM SOLUTION		X			X	X						X													22
30. OLEFINS		X	X																						30
31. PARAFFINS																									31
32. AROMATIC HYDROCARBON MIXTURES			X																						32
33. MISCELLANEOUS HYDROCARBON MIXTURES			X																						33
34. ESTERS		X	X																						34
35. VINYL HALIDES			X																				X		35
36. HALOGENATED HYDROCARBONS																									36
37. NITRILES		X																							37
38. CARBON DISULFIDE						X	X																		38
39. SULFOLANE																									39
40. GLYCOL ETHERS		X										X													40
41. ETHERS		X	X																						41
42. NITROCOMPOUNDS					X	X	X	X	X																42
43. MISCELLANEOUS WATER SOLUTIONS		X										X													43
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22			

1994 Cargo Compatibility Chart, USCG 46 CFR part 150

250th American Chemical Society National Meeting & Exposition, Boston MA, Aug 2015



CRW 3.0/CAMEO

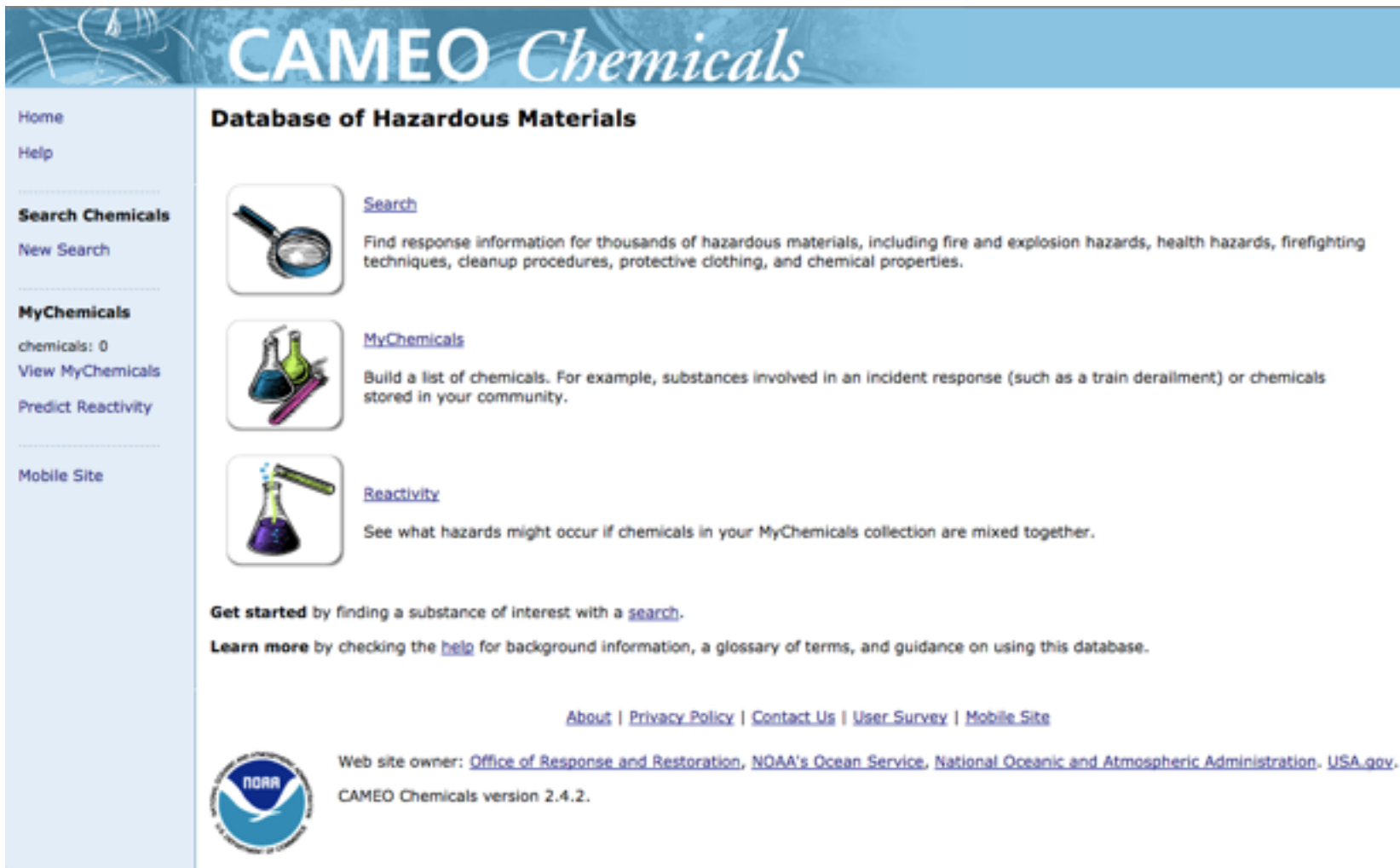
	1. Acetals, Ketals, Hemiacetals, and Hemiketals	2. Acid Halides, Sulfonyl Halides, and Chloroformates	3. Acids, Carboxylic	4. Acids, Strong Non-oxidizing	5. Acids, Strong Oxidizing	6. Acids, Weak
1. Acetals, Ketals, Hemiacetals, and Hemiketals						
2. Acid Halides, Sulfonyl Halides, and Chloroformates	Incompatible					
3. Acids, Carboxylic	Compatible	Incompatible				
4. Acids, Strong Non-oxidizing	Caution	Incompatible	Incompatible			
5. Acids, Strong Oxidizing	Incompatible	Incompatible	Incompatible	Incompatible		
6. Acids, Weak	Compatible	Incompatible	Compatible	Caution	Incompatible	
7. Acrylates and Acrylic Acids	Caution	Caution	Caution	Incompatible	Incompatible	Caution

1998 J. Farr *et al* "New Program for Chemical Compatibility" Chemical Health and Safety 5

250th American Chemical Society National Meeting & Exposition, Boston MA, Aug 2015



CAMEO: Computer-Aided Management of Emergency Operations



The screenshot shows the CAMEO Chemicals website. At the top, there is a blue header with the text "CAMEO Chemicals" in white. Below the header is a navigation menu on the left side with links for "Home", "Help", "Search Chemicals", "New Search", "MyChemicals", "chemicals: 0", "View MyChemicals", "Predict Reactivity", and "Mobile Site". The main content area is titled "Database of Hazardous Materials" and features three main sections: "Search", "MyChemicals", and "Reactivity". Each section has an icon and a brief description. The "Search" section includes a magnifying glass icon and text about finding response information. The "MyChemicals" section includes an icon of chemical flasks and text about building a list of chemicals. The "Reactivity" section includes an icon of a flask being poured into and text about hazards from mixing chemicals. At the bottom of the main content area, there are links for "About", "Privacy Policy", "Contact Us", "User Survey", and "Mobile Site". Below these links is the NOAA logo and text identifying the website owner as the Office of Response and Restoration, NOAA's Ocean Service, National Oceanic and Atmospheric Administration, USA.gov, and the version as CAMEO Chemicals version 2.4.2.

CAMEO Chemicals

Database of Hazardous Materials

Search
Find response information for thousands of hazardous materials, including fire and explosion hazards, health hazards, firefighting techniques, cleanup procedures, protective clothing, and chemical properties.

MyChemicals
Build a list of chemicals. For example, substances involved in an incident response (such as a train derailment) or chemicals stored in your community.


Reactivity
See what hazards might occur if chemicals in your MyChemicals collection are mixed together.

Get started by finding a substance of interest with a [search](#).

Learn more by checking the [help](#) for background information, a glossary of terms, and guidance on using this database.

[About](#) | [Privacy Policy](#) | [Contact Us](#) | [User Survey](#) | [Mobile Site](#)

Web site owner: [Office of Response and Restoration, NOAA's Ocean Service, National Oceanic and Atmospheric Administration, USA.gov](#).
CAMEO Chemicals version 2.4.2.



<http://cameochemicals.noaa.gov/>



[Click here](#) to find out more about Hazmat Navigator

QUICK

ADVANCED

STRUCTURE

INDEX

Hazmat Navigator is a chemical safety database based on Bretherick's Handbook of Reactive Chemical Hazards that helps chemists and safety personnel quickly access critical, detailed chemical hazards information.

Enter Chemical Name, CAS# or Molecular Formula

SEARCH

[Click here for Search Tips](#)

Hazmat Navigator to Retire

Hazmat Navigator is set to retire and will close on December 31, 2013. To preserve your work, please print it prior to the closing date.

Thank you for your support and patronage of this application. We have enjoyed serving you.
For any questions contact [Customer Service](#).

Sincerely,
The Hazmat Navigator Team



Carcinogenic Potential

[Arsenic acid](#)
[Arsenic trioxide](#)
[Benzene](#)
[Lead arsenate](#)
[Potassium arsenate](#)
[Sodium arsenite](#)

[See more...](#)

Warning: Hazmat Navigator has only partial information for some compounds. If a compound is not included or if information is not provided, DO NOT assume that the compound is without hazard. Proceed at your own risk.

[Privacy](#) [Terms and Conditions](#)

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<http://www.hazmatnavigator.com/search/quick>

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DESCRIBE COMPABILITY MATRICES IN XML?

Encode in XML format

ARE THEY APPLICABLE?

Statistics on reaction corpus

CASANDRA 1.0 RULE EXPRESSIONS

ContainsComponent

Find a reactant by

name (spelling corrected)

chemical structure (Unique SMILES or InChI)

quantity threshold and normalisation (e.g. > 10 g)

role (e.g. solvent)

ContainsPattern

Find reactants that a SMARTS pattern **hits**

Contains - enables indirection



```
<alert mesg="...">
  <any>
    <containsComponent name="TNT"/>
    <containsComponent name="trinitrotoluene"/>
  </any>
</alert>
```

```
<alert mesg="...">
  <containsPattern name="[NX3](~[OX1])~[OX1]" atLeast="3"/>
</alert>
```

```
<alert mesg="...">
  <all>
    <any>
      <containsComponent name="nitrobenzene"/>
      <containsComponent name="nitromethane"/>
    </any>
    <any>
      <containsComponent name="aluminium chloride"/>
      <containsComponent name="aluminum chloride"/>
      <containsComponent name="AlCl3"/>
    </any>
  </all>
</alert>
```

Self Contained

Implementation independent
Facilitate exchange and reuse

Flexible

Arbitrarily complex expressions

Meta-Information

Description/Message

Citation, Links

Category

Hierarchy



ENCODED REACTIVE GROUPS

- 3 Acids, Carboxylic
- 5 Aldehydes
- 6 Amides and Imides
- 7 Amines, Phosphines, and Pyridines
- 8 Azo, Diazo, Azido, Hydrazine, and Azide Compounds
- 9 Carbamates
- 11 Cyanides, Inorganic
- 12 Thiocarbamate Esters and Salts/Dithiocarbamate Esters and Salts
- 13 Esters, Sulfate Esters, Phosphate Esters, Thiophosphate Esters, and Borate Esters
- 14 Ethers
- 17 Halogenated Organic Compounds
- 18 Isocyanates and Isothiocyanates
- 19 Ketones
- 20 Sulfides, Organic
- 21 Metals, Alkali, Very Active
- 22 Metals, Elemental and Powder, Active
- 23 Metals, Less Reactive
- 26 Nitriles
- 27 Nitro, Nitroso, Nitrate, and Nitrite Compounds, Organic
- 30 Peroxides, Organic
- 31 Phenols and Cresols
- 32 Sulfonates, Phosphonates, and Thiophosphonates, Organic
- 34 Epoxides
- 35 Metal Hydrides, Metal Alkyls, Metal Aryls, and Silanes
- 37 Anhydrides
- 38 Salts, Acidic (dictionary list)**
- 39 Salts, Basic (dictionary list)**
- 40 Acid Halides, Sulfonyl Halides, and Chloroformates
- 42 Organometallics
- 44 Oxidizing Agents (dictionary list)**
- 47 Fluorinated Organic Compounds
- 55 Chlorosilanes
- 58 Siloxanes
- 65 Conjugated Dienes
- 66 Aryl Halides
- 68 Amines, Aromatic
- 69 Nitrate and Nitrite Compounds, Inorganic
- 70 Acetals, Ketals, Hemiacetals, and Hemiketals
- 71 Acrylates and Acrylic Acids
- 72 Phenolic Salts
- 73 Quaternary Ammonium and Phosphonium Salts
- 74 Sulfite and Thiosulfate Salts
- 75 Oximes



REMAINING REACTIVE GROUPS

Planned (17)

1 Acids, Strong Non-oxidizing

2 Acids, Strong Oxidizing

4 Alcohols and Polyols

10 Bases, Strong

16 Hydrocarbons, Aromatic

28 Hydrocarbons, Aliphatic Unsaturated

29 Hydrocarbons, Aliphatic Saturated

33 Sulfides, Inorganic

45 Reducing Agents

46 Non-Redox-Active Inorganic Compounds

51 Nitrides, Phosphides, Carbides, and Silicides

59 Halogenating Agents

60 Acids, Weak

61 Bases, Weak

62 Carbonate Salts

63 Alkynes, with Acetylenic Hydrogen

64 Alkynes, with No Acetylenic Hydrogen

Difficult non-structural categories:

76 Polymerizable Compounds

98 Not Chemically Reactive

99 Insufficient Information for Classification

100 Water and Aqueous Solutions

101 Highly Flammable

102 Explosive

103 Polymerizable

104 Strong Oxidizing Agent

105 Strong Reducing Agent

106 Known Catalytic Activity

107 Water-Reactive

108 Air-Reactive

109 Pyrophoric

110 Decomposes at Elevated Temperatures (<120 deg. C)

111 Peroxidizable Compound

400 Radioactive Material



cameochemicals.noaa.gov/reactivity/documentation/RG5-RG7

Reactivity Predictions (for each pair of reactive groups)

Aldehydes mixed with Amines, Phosphines, and Pyridines

Hazard Predictions

- Exothermic reaction at ambient temperatures (releases heat)
- Reaction may be particularly intense, violent, or explosive

Acetaldehyde reacts violently with amines (MCA Safety Datasheet 43, Manufacturing Chemists' Association, Washington, 1952).

Tertiary amines promote exothermic aldol condensations between aldehydes and/or ketones (Kohlpaintner, C., M. Schulte, J. Falbe, P. Lappe, and J. Weber. 2002. Aldehydes, Aliphatic and Aromatic. In Ullmann's Encyclopedia of Industrial Chemistry. Wiley-VCH Verlag GmbH & Co. KGaA. (Online)).

Hazards involving Acrolein (unsaturated aldehyde):

Acrolein polymerizes explosively on contact with amines (Arntz, D., M. Hopp, S. Jacobi, J. Sauer, T. Ohara, T. Sato, N. Shimizu, G. Prescher, H. Schwind, and O. Weiberg. 2002. Acrolein. In Ullmann's Encyclopedia of Industrial Chemistry. Wiley-VCH Verlag GmbH & Co. KGaA. (Online)).

Ethylenediamine may react violently with acrolein (Lewis, R.J., Sr. 1992. Sax's Dangerous Properties of Industrial Materials, 8th Edition. New York: Van Nostrand Reinhold. pp. 1554.).

Amines such as dimethylamine and triethylamine promote polymerization of acrolein (Urban, P.G. 1995. Bretherick's Handbook of Reactive Chemical Hazards, 5th Edition. Oxford: Butterworth-Heinemann. pp. 417.).



RULE HIERARCHY

rg-5_7 (general)

Aldehydes and **Amines, Phosphines, and Pyridines**

rg-5_7* (specific)

- a. Acetaldehyde reacts violently with **amines**.
- b. **Tertiary amines** promote exothermic aldol condensations between **aldehydes** and/or **ketones**.
- c. Acrolein polymerizes explosively on contact with **amines**.
 - a. Ethylenediamine may react violently with acrolein.
 - b. Amines such as dimethylamine and triethylamine promote polymerization of acrolein.



```
<alert name="rg_5_7" mesg="...">
  <contains ref="aldehydes">
    <contains ref="amines,phosphines,pyridines">
</alert>
```

...

```
<alert name="rg_5_7c" mesg="polymerizes explosively on contact"
  parent="rg_5_7">
  <containsComponent name="acrolein">
  <contains ref="amines">
</alert>
```

```
<alert name="rg_5_7c_a" mesg="may react violently"
  parent="rg_5_7c">
  <containsComponent name="acrolein">
  <containsComponent name="ethylenediamine">
</alert>
```

```
<alert name="rg_5_7c_b" mesg="prompts polymerization"
  parent="rg_5_7c">
  <containsComponent name="acrolein">
  <any>
    <containsComponent name="dimethylamine">
    <containsComponent name="triethylamine">
  </any>
</alert>
```

COMPONENT EXPRESSIONS (2.0)

```
<condition name="trialkylboranes">
  <containsComponent>
    <smarts value="[CX4][BX3]([CX4])[CX4]" />
    <not>
      <smarts value="([CX4][BX3]([CX4])[CX4].[!#1!C!X4])" />
    </not>
  </containsComponent>
</condition>
...
<alert name="epa-rg-35_42b"
  msg="Form strongly basic reducing agents (LiBHR3)."
  cite="Sullivan, E. and Wade, R. 1980. Hydrides...">
  <all>
    <containsComponent name="lithium hydride" />
    <contains ref="trialkylboranes" />
  </all>
</alert>
```



1,375 rules (18K lines)

∞ GENERAL COMBINATIONS

∞ semi-automatic

4 297 **incompatible** 191 **caution**

7 SPECIFIC COMBINATIONS

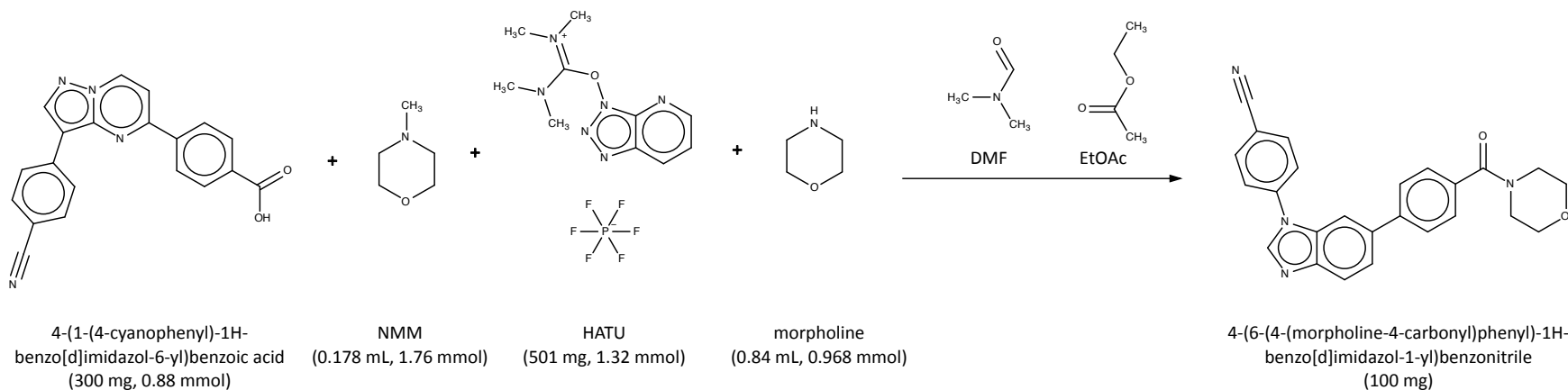
∞ manual

∞ 744 **incompatible** 143 **caution**

1,566,049 USPTO REACTIONS

US20150038506A1 [paragraph:943]

[0943] Step 7: To a solution of 4-(1-(4-cyanophenyl)-1H-benzo[d]imidazol-6-yl)benzoic acid 6 (300 mg, 0.88 mmol) in DMF (5 mL) was added NMM (0.178 mL, 1.76 mmol) followed by HATU (501 mg, 1.32 mmol) at rt and the solution was stirred for 30 min. Morpholine (0.84 mL, 0.968 mmol) was added to the reaction mixture and stirring was continued for 16 h. The reaction mixture was diluted with EtOAc and washed with water and brine solution. The organic layer was dried over anhydrous Na₂SO₄ and concentrated under reduced pressure to obtain crude product. The crude product was purified by preparative HPLC to afford 4-(6-(4-(morpholine-4-carbonyl)phenyl)-1H-benzo[d]imidazol-1-yl)benzonitrile (100 mg, 27%, AUC HPLC 95.9%) as an off-white solid; m.p. 207-210° C.; ¹H NMR (400 MHz, CDCl₃) δ (ppm): 8.18 (s, 1H), 7.98-7.92 (m, 3H), 7.72 (d, J=6.6 Hz, 3H), 7.66-7.61 (m, 3H), 7.51 (d, J=7.9 Hz, 2H), 3.90-3.40 (m, 8H); MS (ESI) m/z 409.15 [C₂₅H₂₀N₄O₂+H]⁺.



nextmovesoftware.com/leadmine.html

nextmovesoftware.com/blog/2014/02/

250th American Chemical Society National Meeting & Exposition, Boston MA, Aug 2015



WARNINGS OVERVIEW

1,431,165 (91%) reactions flagged in **3h3m12s**

7 ms avg per reactions (**142 s⁻¹**)

6,200,046 incompatibles

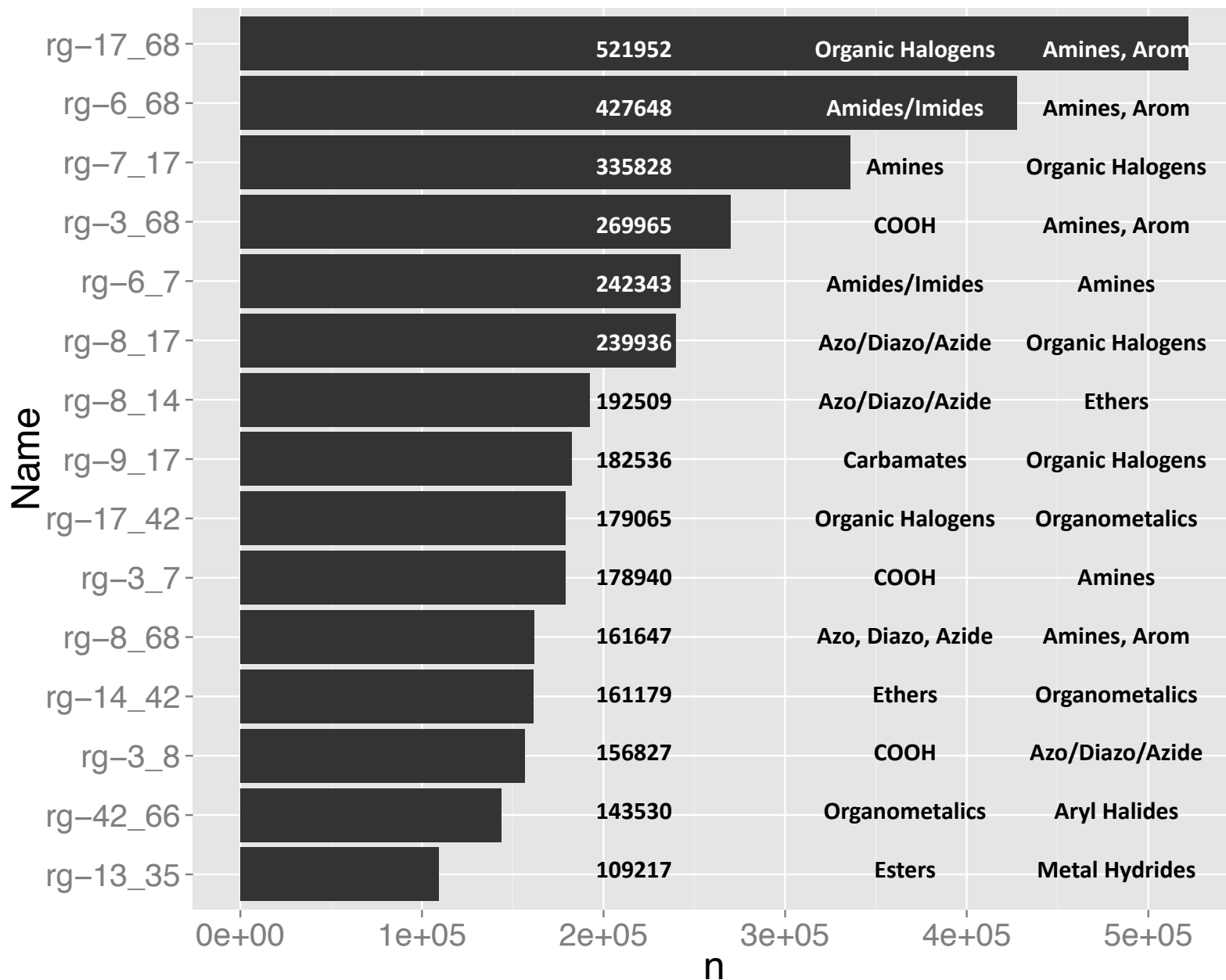
1,477,142 specific in 642,649 (**41%**) reactions

3,247,847 cautions

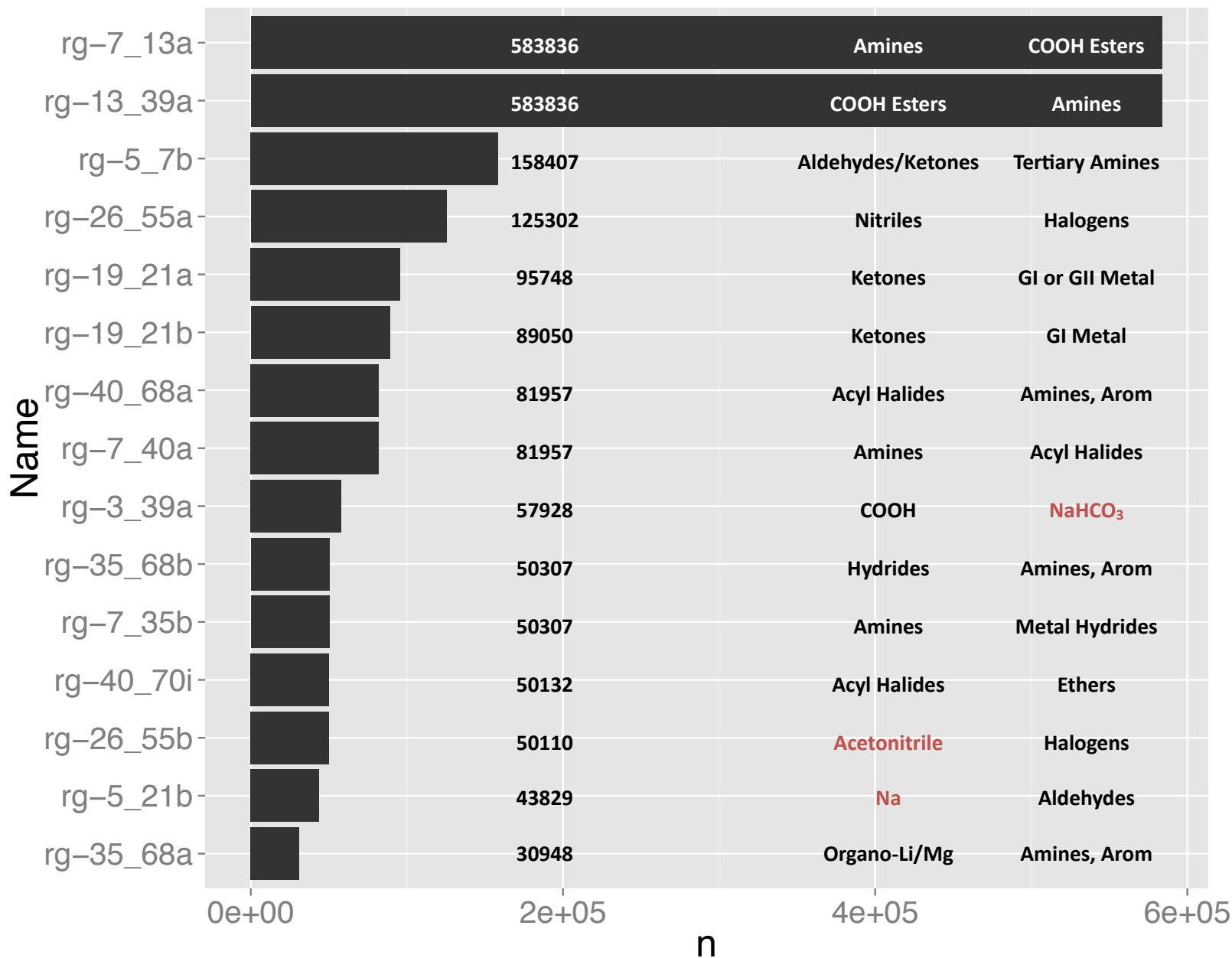
1,194,938 specific in 600,209 (**38%**) reactions



TOP 15 GENERAL INCOMPATIBILITIES



TOP 15 SPECIFIC INCOMPATIBILITIES



INFORMATION OVERLOAD

1. Scope/Structure of CRW/CAMEO

for emergency responders rather than experimentalists

2. Coarse Hazard Level

dimethylmercury and methanol pictograms:

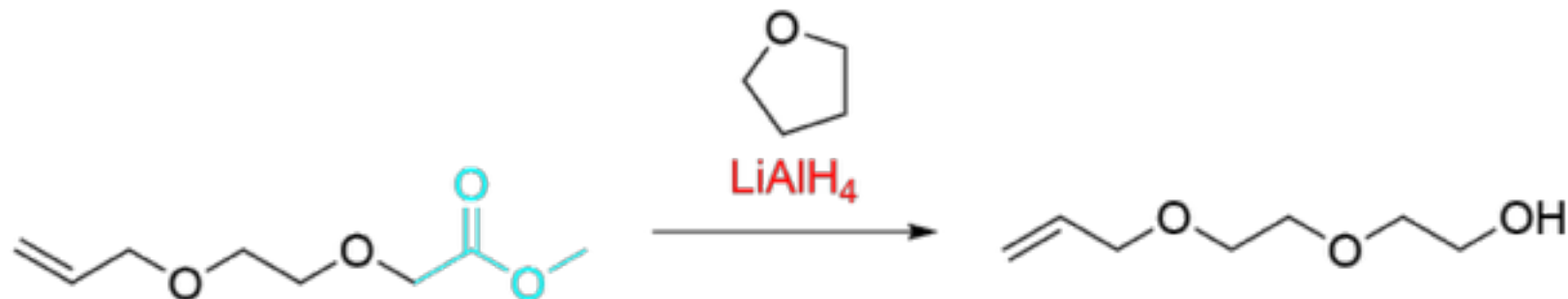


3. Classification accuracy

Loose structural patterns

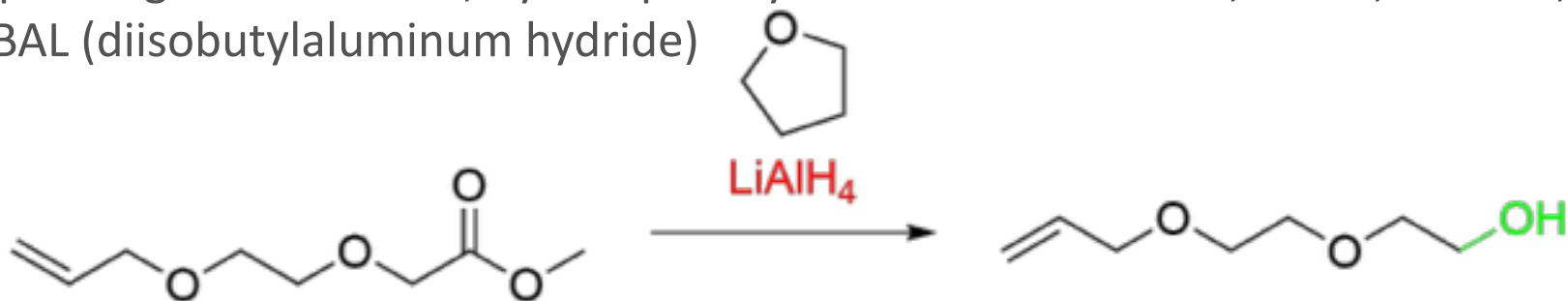


US20110306771A1 [paragraph:0056]



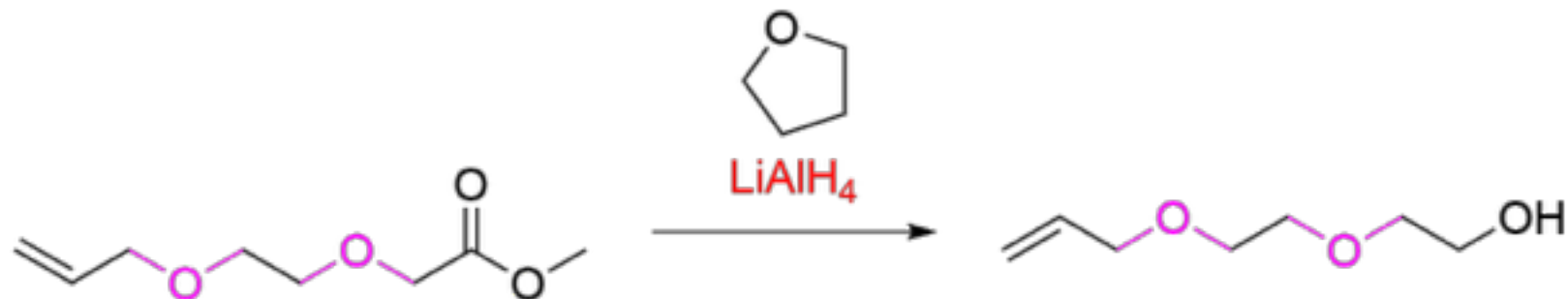
rg-13_35e esters can be reduced to alcohols with complex metal hydrides, especially **lithium aluminum hydride**.

rg-13_35b carboxylic acid esters can be reduced to aldehydes or alcohols, depending on conditions, by complex hydrides such as **LiAlH_4** , LiBH_4 , NaAlH_4 , or DIBAL (diisobutylaluminum hydride)



rg-35_70d hydrides react spontaneously and irreversibly with proton donors, including **alcohols**, evolving flammable H_2 gas





rg-14_42 solutions of molybdenum hexacarbonyl (42?) in diethylether (14) can explode after standing in air for an extended period. Chromium hexacarbonyl in diethylether may behave the same way

rg-35_42 the interaction between tetravinyllead (42?) and diborane (35) is explosively violent at ambient temperature.

14: Ethers

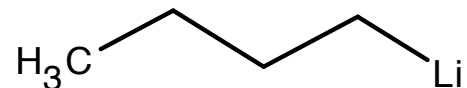
35: Metal Hydrides, Metal Alkyls, Metal Aryls, and Silanes

42: Organometallics (previously just matched as 'has metal')

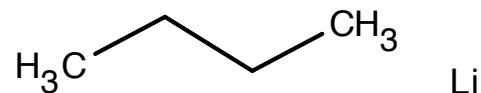


ORGANOMETALIC STRUCTURAL PATTERN

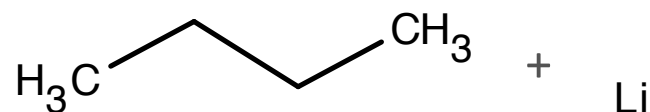
[#6]–[#M] carbon–metal bond



[#6].[#M] carbon and metal



[#M] metal



[#M] = [!#1!#2!#5!#6!#7!#8!#9!#10!#14!#15!#16!#17!
#18!#35!#36!#53!#54!#85!#86!#117!#118]



CAMEO COMPLETENESS

Reactivity Predictions (for each pair of reactive groups)

Amides and Imides mixed with Amines, Aromatic

Hazard Predictions

- Reaction products may be flammable
- Reaction liberates gaseous products and may cause pressurization
- Reaction products may be toxic

Thionamides may react with amines, anilines, hydrazine, and ammonium hydroxide to liberate toxic and flammable H₂S gas (Smith, P. A. S., Open-Chain Nitrogen Compounds, Vol. I. New York: W. A. Benjamin, Inc., 1965, pp. 162).

Potential Gas Byproducts

- Hydrogen Sulfide (H₂S)

<http://cameochemicals.noaa.gov/reactivity/documentation/RG6-RG68>



CAMEO INCONSISTENCIES

Reactivity Predictions (for each pair of reactive groups)

Nitriles mixed with

Chlorosilanes

Hazard Predictions

- Reaction liberates gaseous products and may cause pressurization
- Exothermic reaction at ambient temperatures (releases heat)
- Polymerization reaction may become intense and may cause pressurization
- Reaction products may be toxic

Halogens may initiate polymerization of acrylonitrile, even at reduced temperatures (MCA Case History No. 1214, Case Histories of Accidents in the Chemical Industry, Manufacturing Chemists' Association, Washington.).

Nitriles may react with the halogens to liberate toxic HX gases (Smith, P. A. S., Open-Chain Nitrogen Compounds, Vol. I. New York: W. A. Benjamin, Inc., 1965, pp. 218).

Potential Gas Byproducts

- Hydrogen Halide (HX)

<http://cameochemicals.noaa.gov/reactivity/documentation/RG26-RG55>



Reactivity Predictions (for each pair of reactive groups)

Amines, Phosphines, and Pyridines mixed with Halogenated Organic Compounds

Hazard Predictions

- Reaction liberates gaseous products and may cause pressurization
- Exothermic reaction at ambient temperatures (releases heat)
- Reaction may be particularly intense, violent, or explosive
- Reaction products may be toxic

Ethylenediamine reacts violently with ethylene chlorohydrin (Lewis, R.J., Sr. 1992. Sax's Dangerous Properties of Industrial Materials, 8th Edition. New York: Van Nostrand Reinhold. pp. 1554.).

Trimethylamine may react with RX compounds to form (CH₂)NR and halogenated methanes (Rodd, E. H, Ed. Chemistry of Organic Compounds. New York: Elsevier Publishing Company, 1951. Vol. I pp. 380).

Ethylphosphine explodes on contact with chlorine, bromine or fuming nitric acid, and inflames with conc. acid. (Fire and Explosion Risks, von Schwartz, E., London, Griffin, 1918, p. 324-325)

Aniline, dimethyl amine and pyridine incandesce on contact with fluorine. (Hoffman, C. J., Chem. Rev., 1962, 62, 12)

Common halogenated hydrocarbons (CH₂Cl₂, CHCl₃, etc.) incompatibility with amines is a well-known reactivity issue in the chemical industry.

Common halogenated hydrocarbons (CH₂Cl₂, CHCl₃, etc.) incompatibility with amines is a well known reactivity issue in the chemical industry.

Potential Gas Byproducts

- Halocarbons

<http://cameochemicals.noaa.gov/reactivity/documentation/RG17-RG7>



Reactivity Predictions (for each pair of reactive groups)

Metal Hydrides, Metal Alkyls, Metal Aryls, and Silanes mixed with Amines, Aromatic

Hazard Predictions

- Reaction products may be corrosive
- Reaction products may be explosive or sensitive to shock or friction
- Reaction products may be flammable
- Reaction liberates gaseous products and may cause pressurization
- Exothermic reaction at ambient temperatures (releases heat)

1) Amines may react with organolithium and organomagnesium reagents to liberate flammable hydrocarbon gases.

- Carey, Francis. "Organic Chemistry", 5th Edition, Chpt. 14. Accessed at:
<http://www.chem.ucalgary.ca/courses/351/Carey5th/Ch14/ch14-1.html#Reactivity>

2) **Hydrides** react spontaneously and irreversibly with amines, evolving flammable H₂ gas.

- Rittmeyer, P., U. Wietelmann. 2002. Hydrides. In Ullmann's Encyclopedia of Industrial Chemistry. Wiley-VCH Verlag GmbH & Co. KGaA. (Online) - Sullivan, E. and Wade, R. 1980. Hydrides. Kirk-Othmer Encyclopedia of Chemical Technology, 3rd ed. John Wiley & Sons, Inc.

3) Aromatic amines react with lithium aluminum hydride to form azo compounds, which are potentially explosive.

- Cartolano, A. R. and Vedage, G. A. 2004. Amines by Reduction. Kirk-Othmer Encyclopedia of Chemical Technology. (Online)

4) Sodium hydride reacts with amines to form corrosive and strongly basic sodium amide salts.

- Klemm, A., Hartmann, G. and Lange, L. 2000. Sodium and Sodium Alloys. Ullmann's Encyclopedia of Industrial Chemistry. (Online)

Potential Gas Byproducts

- Hydrogen (H₂)
- Hydrocarbons

<http://cameochemicals.noaa.gov/reactivity/documentation/RG68-RG35>



CONCLUSIONS

Able to encode many chemical incompatibility matrices in **Cassandra's** self contained XML rule format

real-time alerting (ELN interaction) even with the moderately large rule set

v2.0: Markush like queries, Custom properties

CAMEO is an **excellent** resources for hazard information

Still room for improvement and reorganisation:

wiki, ontology, self-organising hierarchy, citations

Repurposing for experimentalist is feasible given dedicate manual curation

Validation *corpus* are relevant hazards identified/missed



FUTURES

Classification And Labelling Requirements For Hazardous Substances And Mixtures

Table 2.6.1

Category	Flash Point	Initial Boiling Point
GHS 1 Flammable Liquids	< 23 °C	≤ 35 °C
GHS 2 Flammable Liquids	< 23 °C	> 35 °C
GHS 3 Flammable Liquids	≥ 23 °C ≤ 60 °C	

Liquid:

- vapour pressure ≤ 300 kPa at 50 °C
- not completely gaseous at 20 °C at a standard pressure 101,3 kPa
- (initial) melting point ≤ 20 °C at a standard pressure 101,3 kPa



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<http://nextmovesoftware.com>

Slides will be available:

<http://www.slideshare.net/NextMoveSoftware>

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