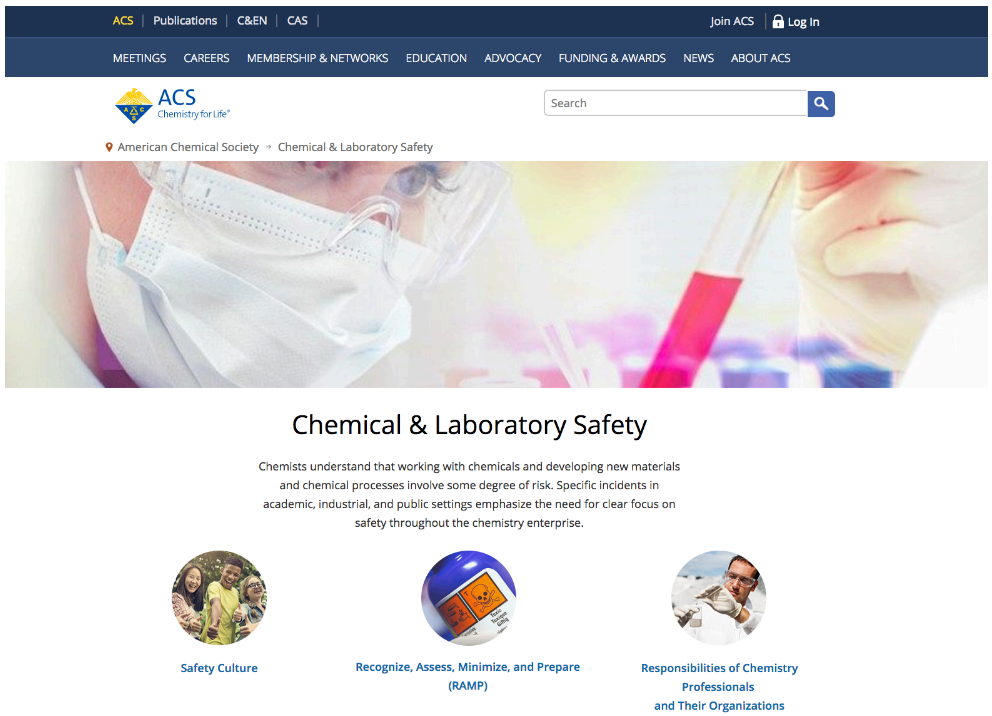
acs.org/safety



Modeling Terminology *for* Chemical Safety

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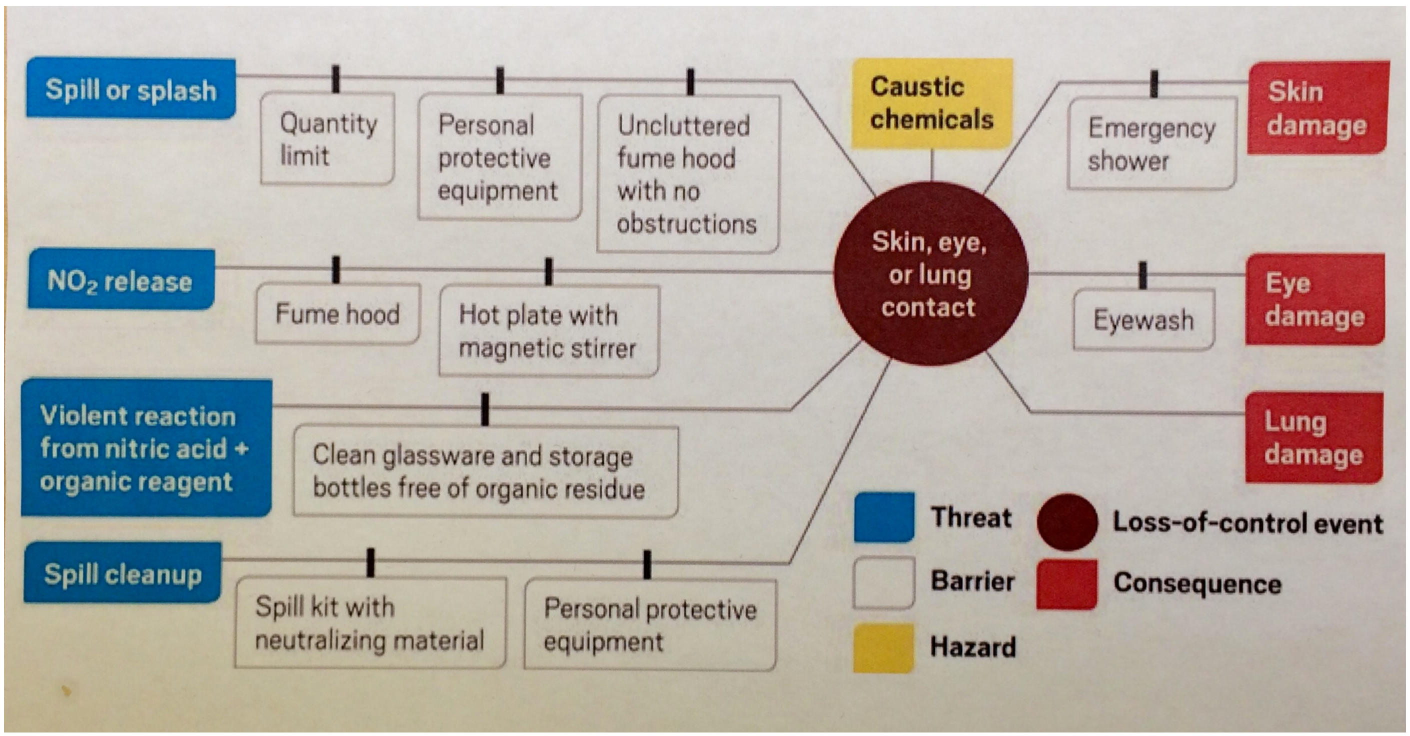
Work begun at VoCamp, University of Maryland, 2016.11.29/30

Collaborators: Gary Berg-Cross, Evan Bolton, Ahmed Eliesh,
Chris Jakober, Phil Painter, Ralph Stuart

Lab Safety Model for Reported Incidents



Data from Reported Incident Strings

1. Arsine, phosphine, and tetraborane are all oxidized explosively by fuming nitric acid.

2. Phosphine, hydrogen sulfide, and selenide all ignite when fuming nitric acid is dripped into the gas.

3. Hydrogen telluride ignites with cold concentrated nitric acid, sometimes exploding.

- Substances
- Outcomes
- Consequences
- Conditions
- Operations
- Apparatus/ equipment

https://pubchem.ncbi.nlm.nih.gov/compound/nitric_acid

Use cases

- Support core questions in the risk assessment decision process
  - Conceptual analysis of research laboratory procedures
  - Identification of prevention and mitigation controls for multiple hazard types
  - Incident analysis including threats, consequences, and loss of control
- Annotate collections of chemical incident data and other text-based information relevant to chemical health and safety
- Support use of hazard recognition and evaluation tools (RAMP)
- Inform templates for further reporting and build knowledge-base

Decision Process For Safety Assessment

RAMP: goal is to identify what and how to implement safety controls (mitigation) for a particular chemical scenario:

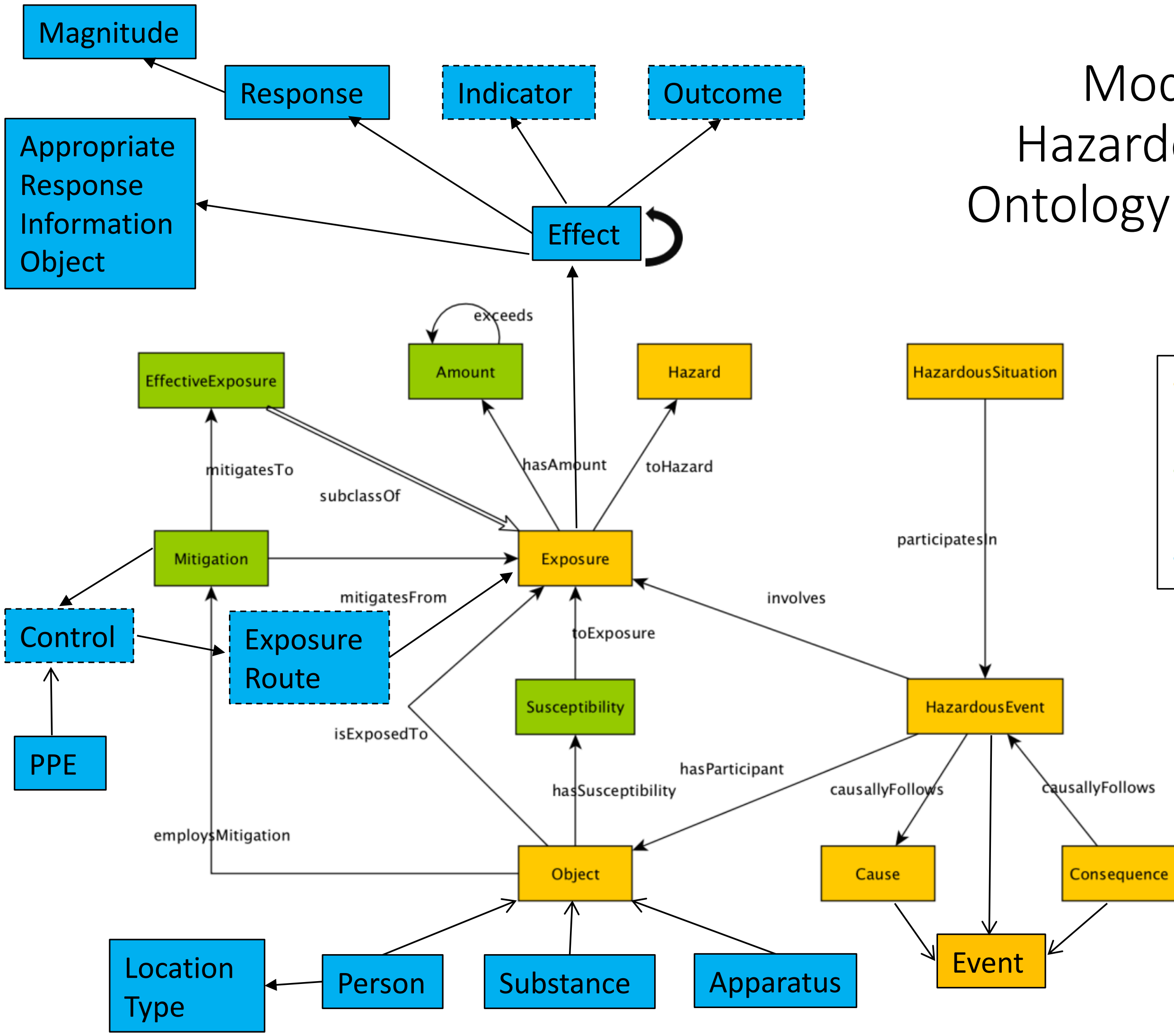
1. **R**ecognize Hazards – chemical disposition, process (and players)
2. **A**ssess Risk – connecting factors (dispositions + process + conditions)
3. **M**anage Controls – determine equipment, procedures
4. **P**repare for Emergency – equipment, procedures, personnel

Core Chemical Safety Queries

1. What substances meet a given set of criteria for hazard properties?
2. What is the consequence of exposing one particular substance to another under a particular condition?
3. What conditions and tasks are associated with hazardous events for a given set of substances?
4. What are the exposure routes of substances used or generated and what controls protect these routes?
5. What mitigation strategies could be used to ameliorate the effect of exposure to a particular hazard?

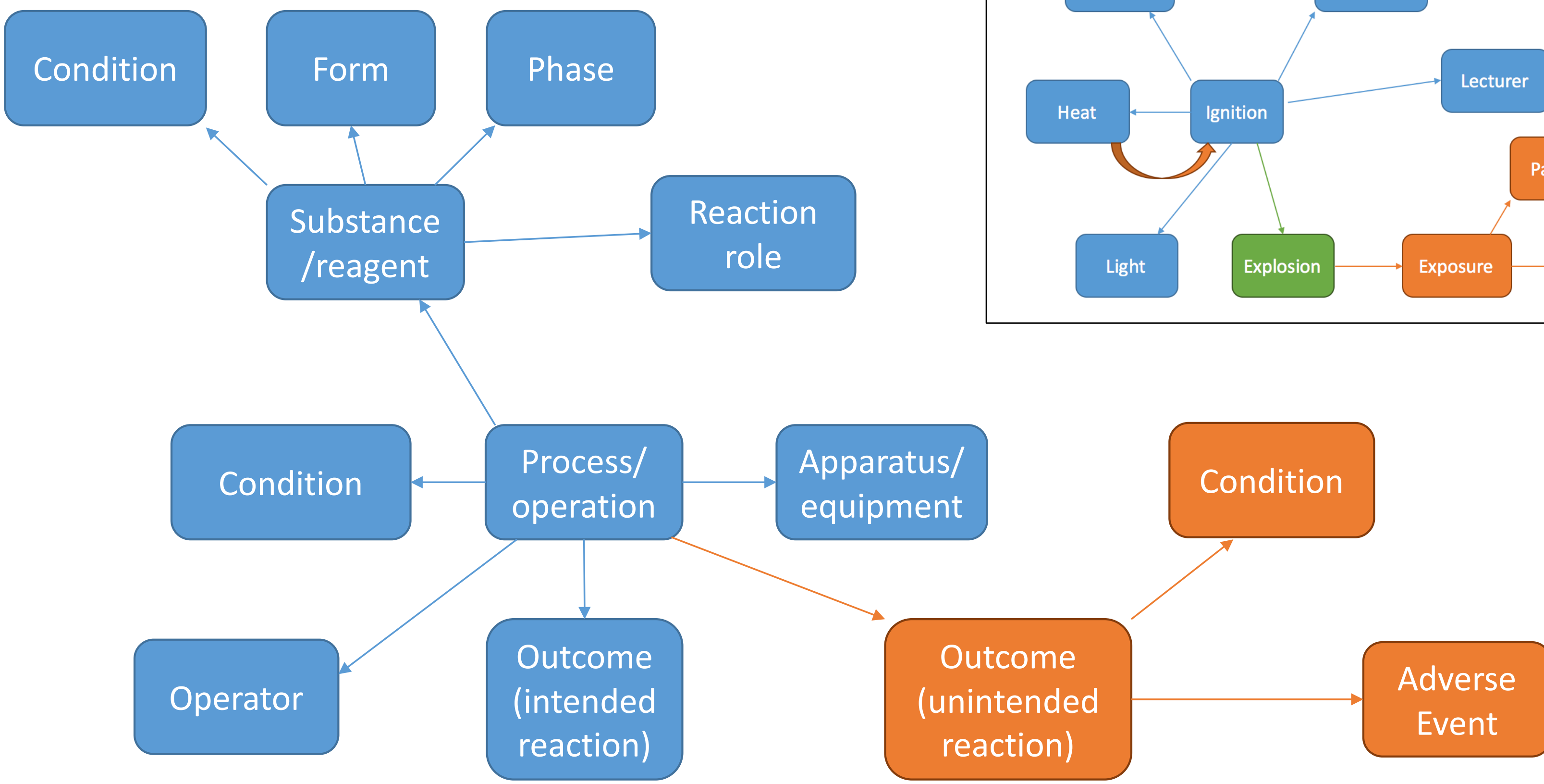
*based on ACS CCS Safety Advisory Panel core questions, 2016

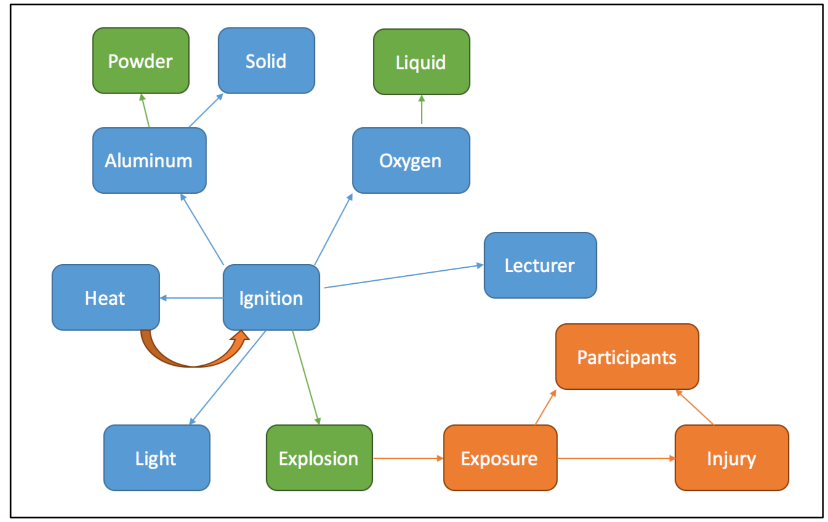
Modifying the Hazardous Situation Ontology Design Pattern



- Lawrynowicz and Lawniczak. 2015
- Cheatham et al. 2016
- VoCamp 2016

Experiment Process Factors





Analyze Data
(Chemical Procedure parser)

UNIVERSITY OF CAMBRIDGE

ChemicalTagger

University of Cambridge > Department of Chemistry > Unilever Centre for Molecular Science Informatics

To a stirred solution of 4-hydroxypiperidine (0.97 g , 9.60 mmol) in anhydrous dimethylformamide (20 mL) at 0 °C was added 1-(bromomethyl)-4-methoxybenzene (1.93 g , 9.60 mmol) and triethylamine (2.16 g , 21.4 mmol) . The reaction mixture was then warmed to room temperature and stirred overnight . After this time the mixture was concentrated under reduced pressure and the resulting residue was dissolved in ethyl acetate (40 mL) , washed with water (20 mL) and brine (20 mL) before being dried over sodium sulfate . The drying agent was filtered off and the filtrate concentrated under reduced pressure . The residue obtained was purified by flash chromatography (silica gel , 0-5 % methanol / methylene chloride) to afford 1-(4-methoxybenzyl)piperidin-4-ol as a brown oil (1.70 g , 80 %) .

Actions:
Filter Yield Heat Wash Concentrate Dry Dissolve Add Stir Purify

Conditions:
TempPhrase TimePhrase

Molecules:
Other Solvent

Phrases:
PrepPhrase NounPhrase VerbPhrase

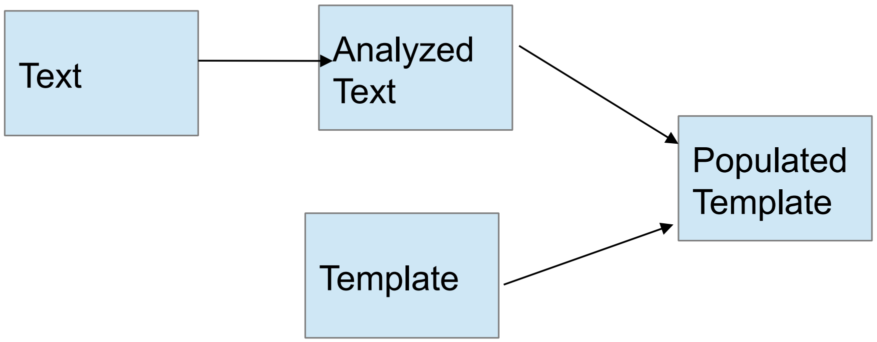
Quantitative_Terms:
Quantity

View XML

Links
- Web Interface
- Instructions
- Documentation
- Publication
- BitBucket Project
- Downloads

Accessibility | Privacy

Safety Report to Structured Data

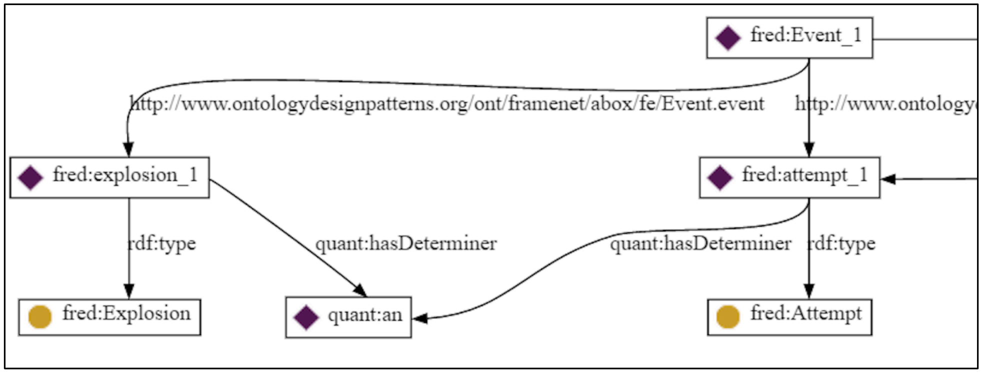


Start with free text, subjected to NLP analysis and harmonized with Safety Template Model

•* incident
-- ActionPhrase : [NN,interact] [RB,vigorously] [RB,exothermally] [IN-IN,in] [NN,presence] [IN-OF,of] [NN-STATE,solid] [TO,to] [VB-YIELD,form]
-- Substance : Chloroform
-- Substance : acetone
-- Substance : potassium hydroxide
-- Substance : calcium hydroxide
-- Substance : 1,1,1-trichloro-2-hydroxy-2-methylpropane

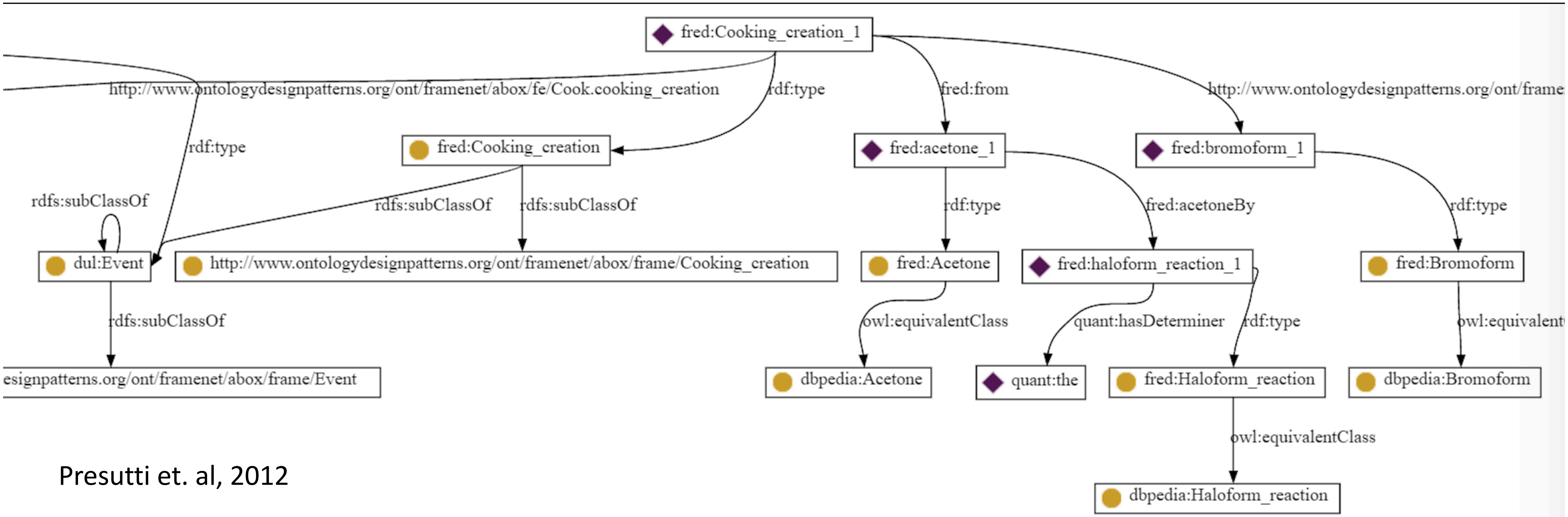
Chloroform and acetone interact vigorously & exothermally in presence of solid potassium hydroxide or calcium hydroxide to form 1,1,1-trichloro-2-hydroxy-2-methylpropane. A laboratory incident involving the bursting of a solvent residues bottle was attributed to this reaction.

Situation: Chemical Incident
Substance : acetone
Substance Role:
Substance Parameter
Form :
Phase : solid
Concentration :
Conditions :
Process/operation: SYNTHESIZE
Objects: Chloroform
Objects: potassium hydroxide
Objects: calcium hydroxide
Objects: 1,1,1-trichloro-2-hydroxy-2-methylpropane
Obejct Role: (base)
Outcome: (exothermal reaction)
Operator:
Reaction: interact
Chain of Events: reaction with



Discourse Representation

"An explosion occurred during an attempt to prepare bromoform from acetone by the haloform reaction."



Presutti et. al, 2012

GOAL: associate patterns of these factors

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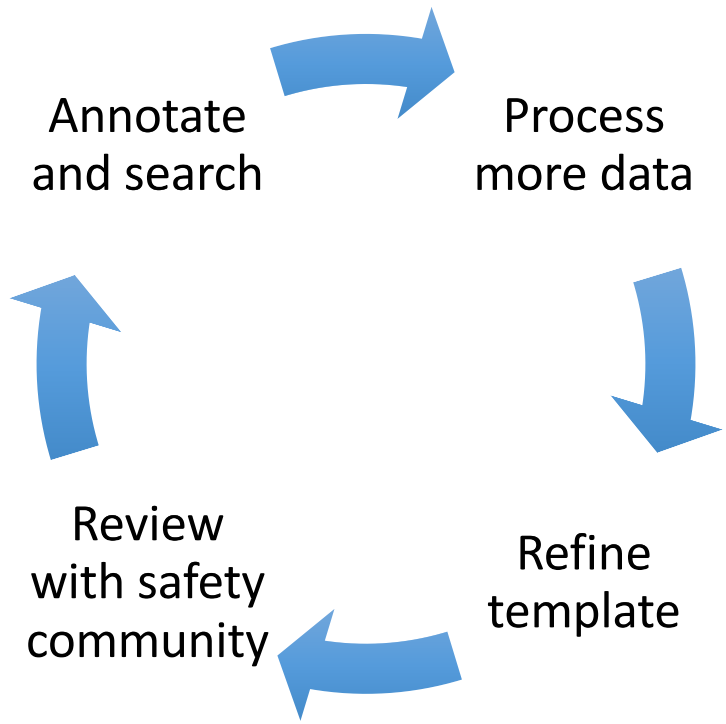
What next?


Annotate
and search
Process
more data
Refine
template
Review
with safety
community