Towards a Pattern-Based Ontology for Chemical Laboratory Procedures

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Content

- Motivation
- The Ontology’s Patterns
- A Worked Example
- Reflections & Future
Motivation

● Risk Assessment
  ○ Data Fusion - Heterogeneous sources

● Post-Mortems
  ○ Incentivize and facilitate entering post-mortems into a system

● Student Use
  ○ Evaluate changes in procedure “on the fly.”
Pattern Overview: Semantic Trajectory

- Trajectory
  - hasSegment
  - hasFix
    - startsFrom
    - endsAt
  - hasAttribute

- Segment
  - hasAttribute

- Fix
  - hasLocation
  - hasSpatialFootprint
  - nextFix
  - atTime
    - subClassOf

- Place
  - Position

- Attribute
  - StartingFix
  - EndingFix

- TimeEntity
Pattern Overview: State Transition
Pattern Overview: Chemical Process
Pattern Overview: Action Patterns
The Incident Report.

5-ethyl-2-methyl-pyridine and 70% nitric acid were placed in a small auto-clave.

They were heated and stirred for 40 minutes.

The emergency vent was opened due to a sudden pressure rise.

A violent explosion occurred 90 seconds later.
● There is still so much to do!
● Many actions haven’t been well-described.
● Extraction/Ingestion workflow
● Accessibility
Conclusion

Thanks!

Questions?