Chemical Reactivity Worksheet

Nicholas Bigelow and Lewis Johnson
University of Washington/NOAA
04/30/2009
CRW: Background

- Software tool for predicting chemical compatibility and hazards using binary combination of reactive groups
- Database of > 5000 common industrial chemicals
- Usable for incident prevention and incident response
New features

• Standalone FileMaker runtime with new user interface
• Majority of reactivity predictions are now documented with literature citations
• Prediction of some possible gaseous products of reactions
• Includes water as a new reactive group
• Ability to create custom databases of chemicals
• Revised hazard statements
Capabilities and Limitations

• CRW does:
  • Predict binary reactions based on reactive groups
  • Make conservative predictions
  • Predict specific gases for some reactions
  • Provide compound-specific info in its database

• CRW does not:
  • Predict trinary or catalytic reactions
  • Predict reaction thermodynamics and kinetics
  • Predict reactions specific to individual compounds (though some info may be available in the database)
CRW2 Demo
Why use CRW?

• Versatile tool for reactivity prediction and information on common industrial chemicals.

• Extensively used over the last 10 years, and much of the compatibility table has been documented.

• Freely available to download:
  • Located under “Software and Data Sets”
Acknowledgements

• Dr. Jim Farr (NOAA)
• Al Hielscher, Brianne Connolly, and Donna Faiferlick (NOAA)
• UW Chemistry Library
• Funding:
  • Center for Chemical Process Safety
  • NOAA
• Conference organizers
• Profs. Bruce Robinson and Rose Ann Cattolico (UW, for letting us out of lab for a couple days)