An active collaboration between faculty and Research Safety to evaluate green chemistry and safety from the bench to the institutional level

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Is green chemistry safer chemistry?

Green chemistry = **Safer chemistry**

Greenness ?

Performance

Safety ?

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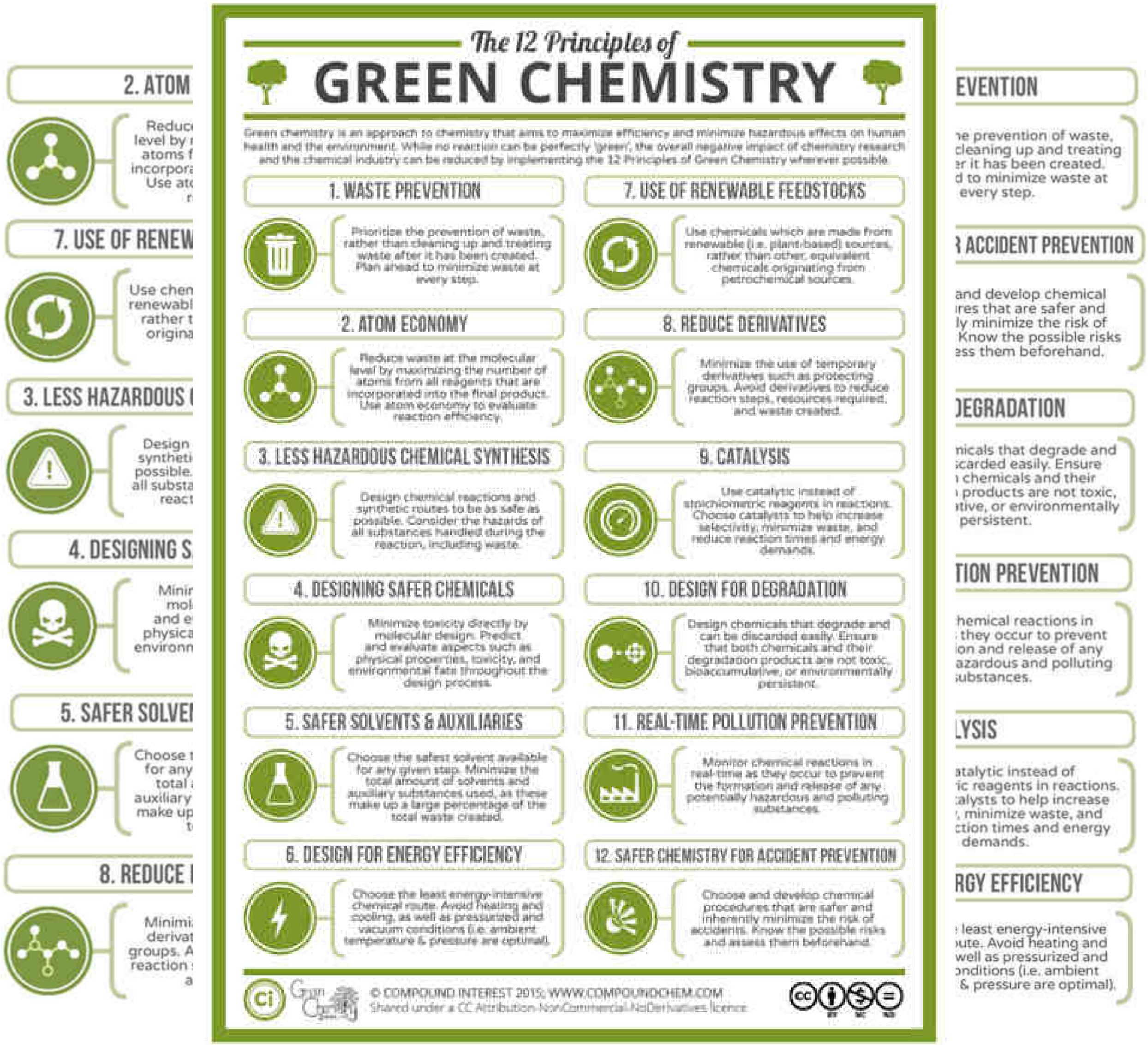
Perspectives lead to different priorities: Green duality



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A holistic approach to green chemistry and safety

Safer chemistry — **Green chemistry**

- Incorporates concepts of scale and perspective
- Incorporates safety concepts by necessity
- Provides student ownership
- Ties green and safety concepts to increased efficiency
- Unique to 'Pilot Plant Clemson'
- Dynamic

Education

Safety

Environmental stewardship

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Green Duality: perspective and scale

Bench

Institution

Flammable Storage

Chemical Storage

Compliance

OSHA Compliance

dhec

NFPA

Incorporating *process* green chemistry and safety

Cradle to grave

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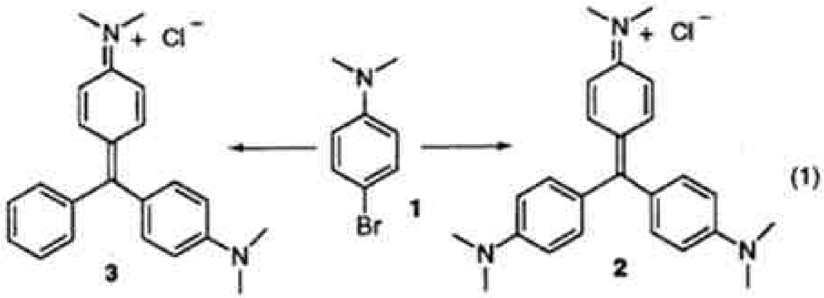
Experiment in green fashion: triphenylmethane dye synthesis

Crystal violet synthesis is our "product"

A Colorful Grignard Reaction

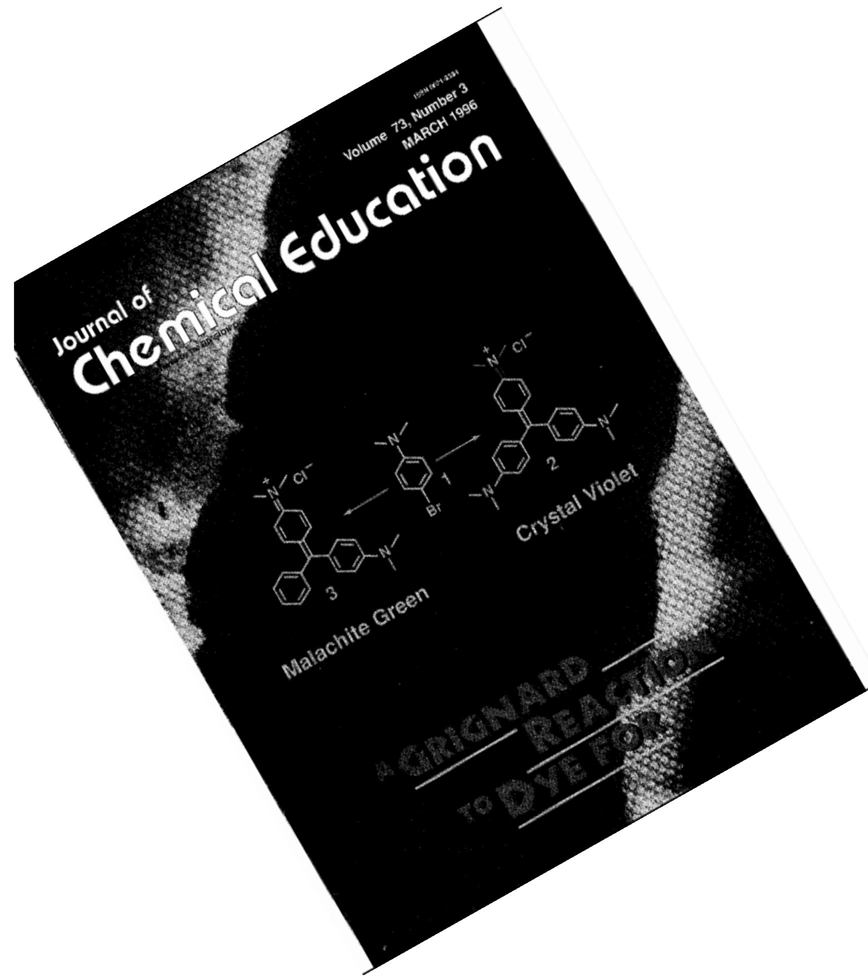
Preparation of the Triarylmethane Dyes from 4-Bromo-*N*,*N*-Dimethylaniline



Malachite Green　　　　　　Crystal Violet

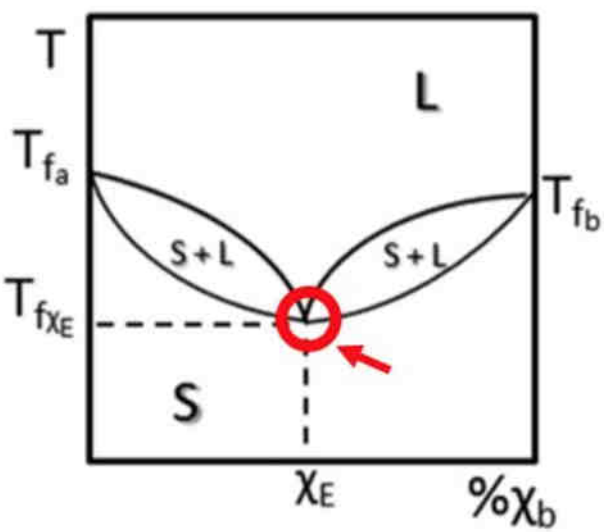
Douglass F. Taber,[1] Robert P. Meagley, and Danielle Supplee
University of Delaware, Newark, DE 19716

Volume 73 Number 3 March 1996 259



Deep Eutectic Solvents (DES) as a greener alternative

- Cheap
- Low Toxicity
- Low Vapor Pressure
- Non flammable
- Tunable
- Derived from renewable sources
- Solvent can also act as catalyst
- Easy to Prepare wit 100% Atom Economy
- Recyclable*

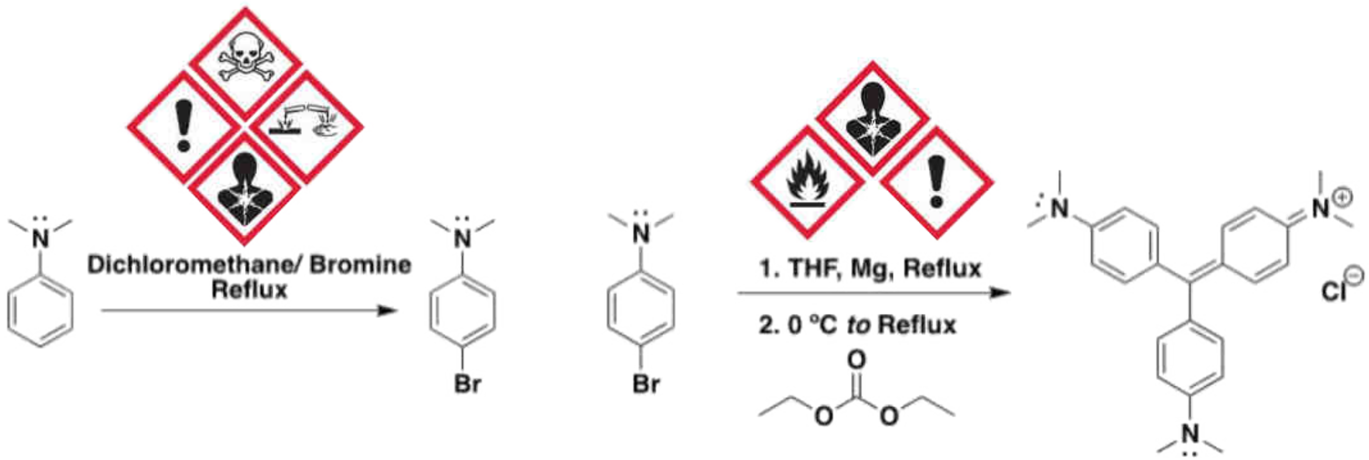


Main types of deep eutectic solvents (Smith et al., 2014).

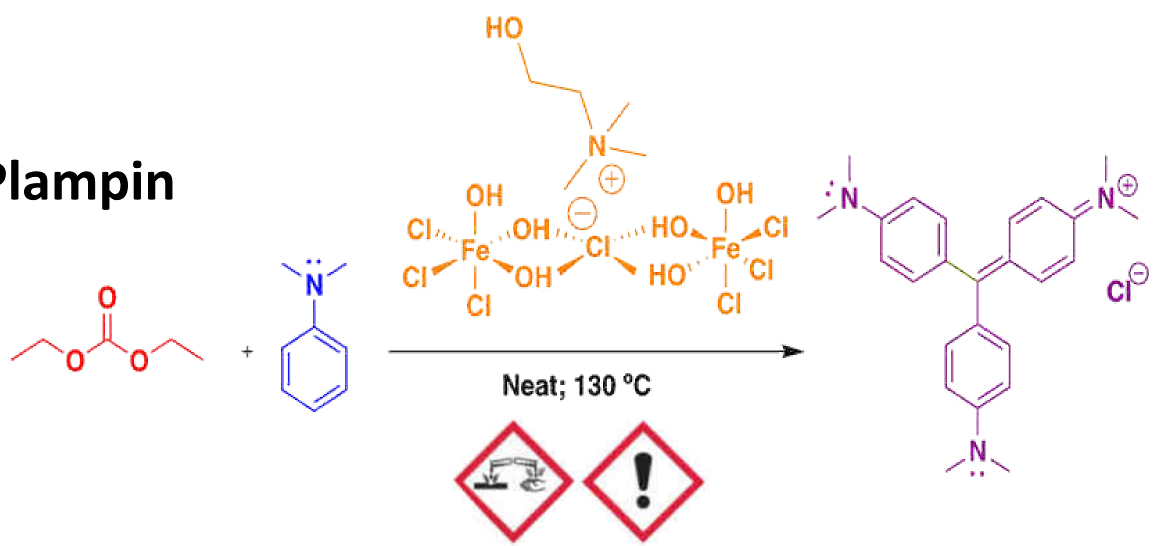
Type	Formula	Term
I	$Cat^+X^-zMCl_x^-$	M: Zn, Sn, Fe, Al, Ga, In
II	$Cat^+X^-zMCl_x \cdot yH_2O$	M: Cr, Co, Cu, Ni, Fe
III	Cat^+X^-zRZ	Z: $CONH_2$, COOH, OH
IV	$MCl_x + RZ = MCl_{x-1}^+ \cdot RZ + MCl_{x+1}$	M: Al, Zn; Z: $CONH_2$, OH

DES based synthesis increases greenness and safety

Taber



Plampin



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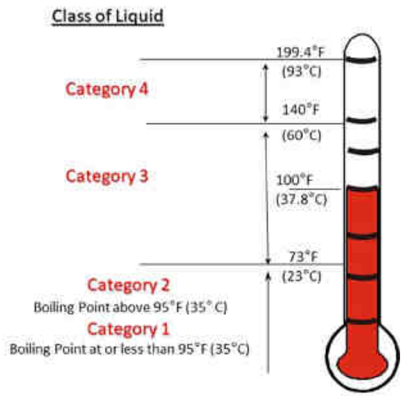
Green metrics don't always scale simply

Bench level	Institutional level
Reaction Yield $$Yield = \frac{actual\ yield}{theoretical\ yield} \times 100\%$$	$$Avg.Yield\ (t)$$
Atom economy $$A.E. = \frac{MW\ \ prod.}{MW\ all\ prod.} \times 100\%$$	$$Inst.A.E.(t) = \frac{\sum MW\ \ prod.}{\sum MW\ all\ prod.} \times 100\%$$
Environmental factor $$E\ factor = \frac{Total\ mass\ waste}{mass\ product}$$	$$\boldsymbol{product \equiv waste}$$

Safety metrics allow quantification of hazards and risk



$$Bench\ Safety\ Value = \frac{1}{\sum BRV}$$

$$Institutional\ Safety\ Value = \frac{1}{\sum IHV}$$

Bench Risk Value (flamı

$$BRV_{Flam} = (total\ mass)R_T$$

Bench Risk Rating (R)

$$R_{Haz} = \frac{1}{n_{Haz}} \qquad R_T = \sum R_{Haz}$$

n_{Haz}

Inst. Hazard Value (stor

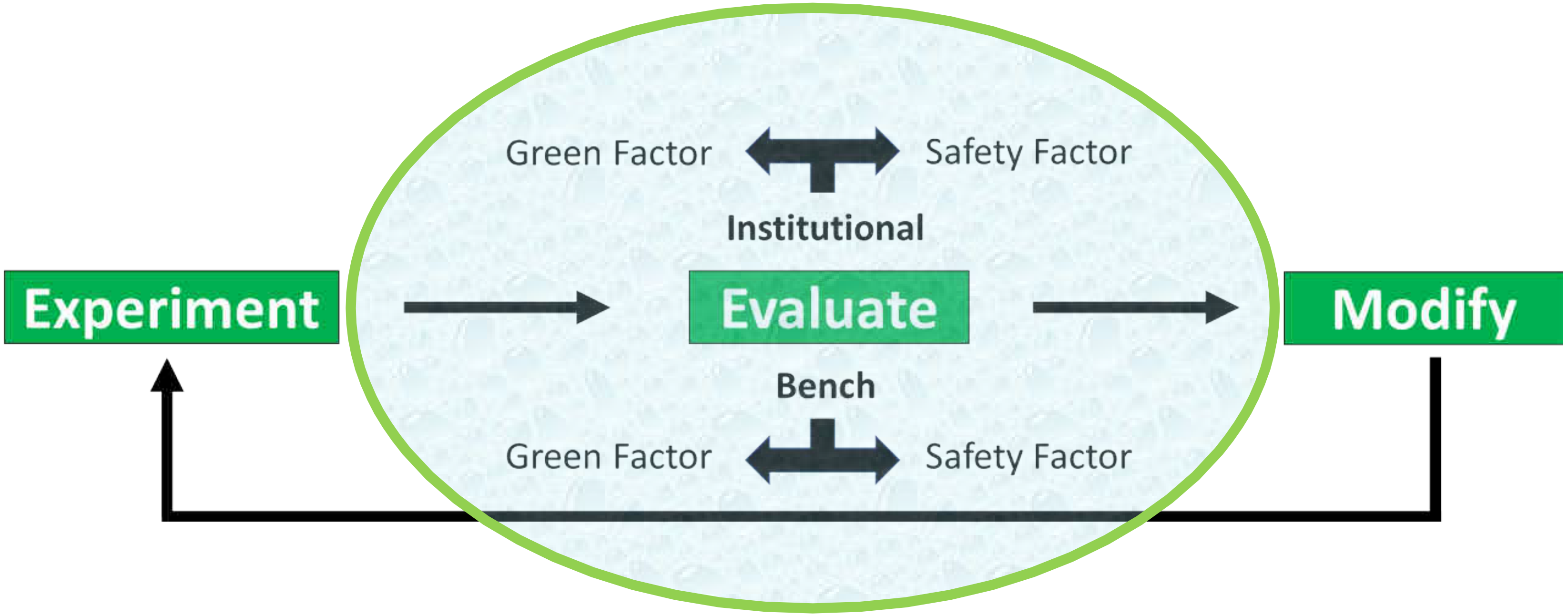
$$IHV_{storage} = (total\ mass)Q_T$$

Inst. Hazard Facto

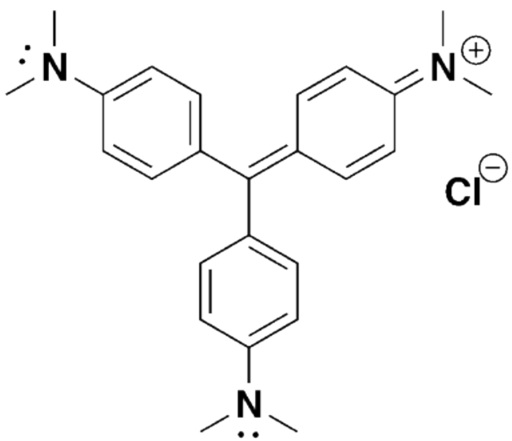
$$Q_{Haz} = \frac{1}{m_{Haz}} \qquad Q_T = \sum Q_{Haz}$$

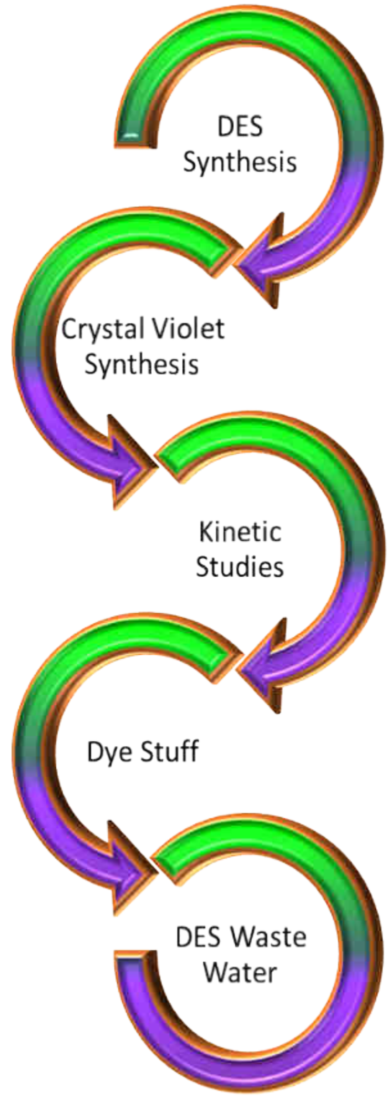
m_{Haz}

Dynamic, iterative modification provides student ownership



Dealing with the atom economy and E-factor problem





Conclusion

- Ongoing partnership between Research Safety and faculty
- Connects green chemistry and safety as a function of scale
- Provides ownership to students through continuous iterations
- Safety concepts and practices incorporated directly

Education

Safety

Environmental stewardship

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SCIENCE

LOCALLY RELEVANT **GLOBALLY IMPACTFUL**