Viikki Teacher Training School,
University of Helsinki

Computational Chemistry in High School Chemistry Education

Constraints and affordances in implementing computational chemistry practices to upper secondary school

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The discussion about “pedagogy first” towards “technology first” determinism.

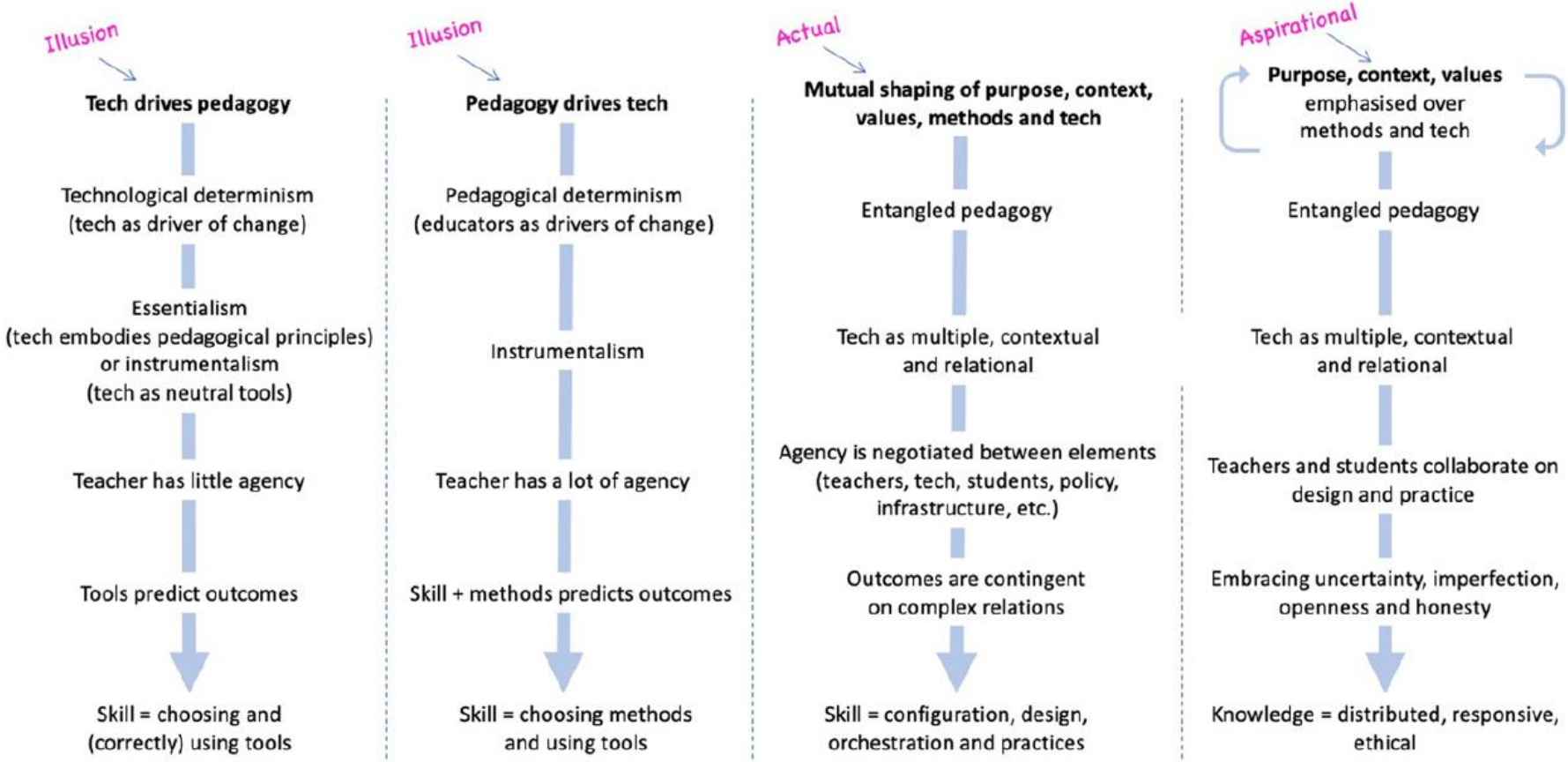
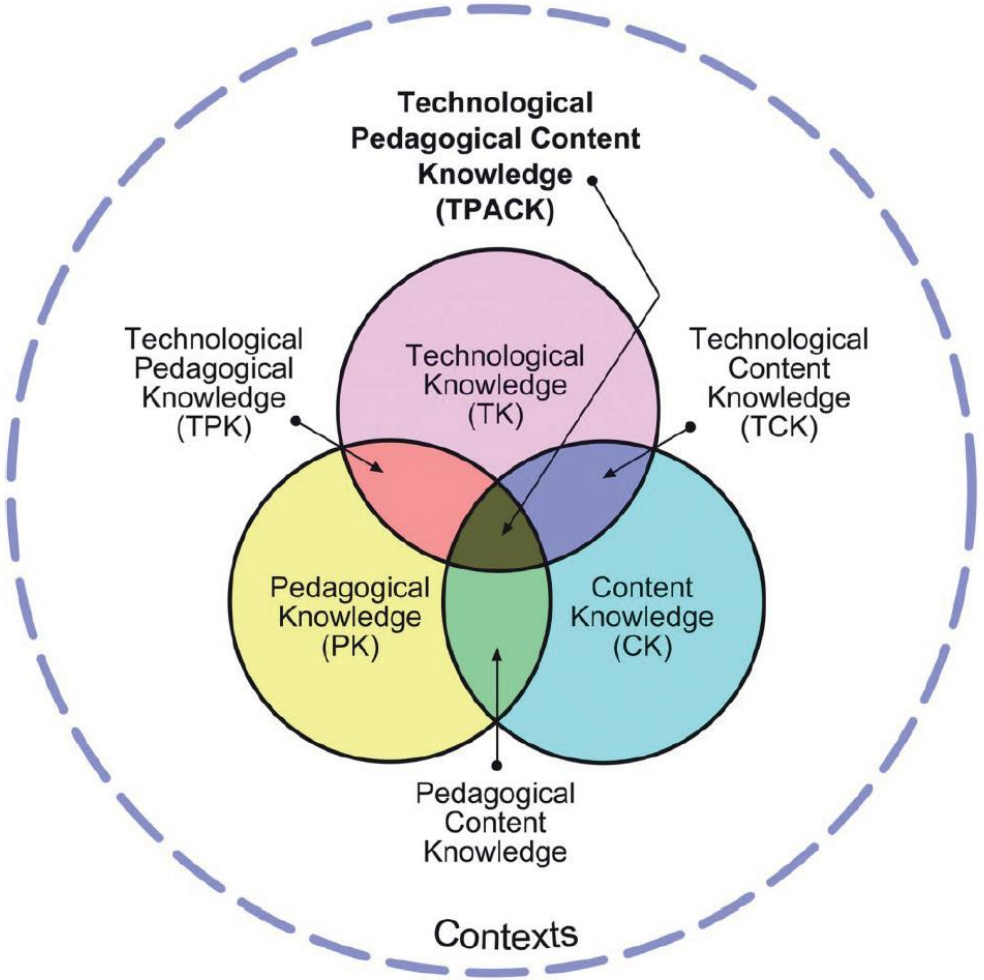


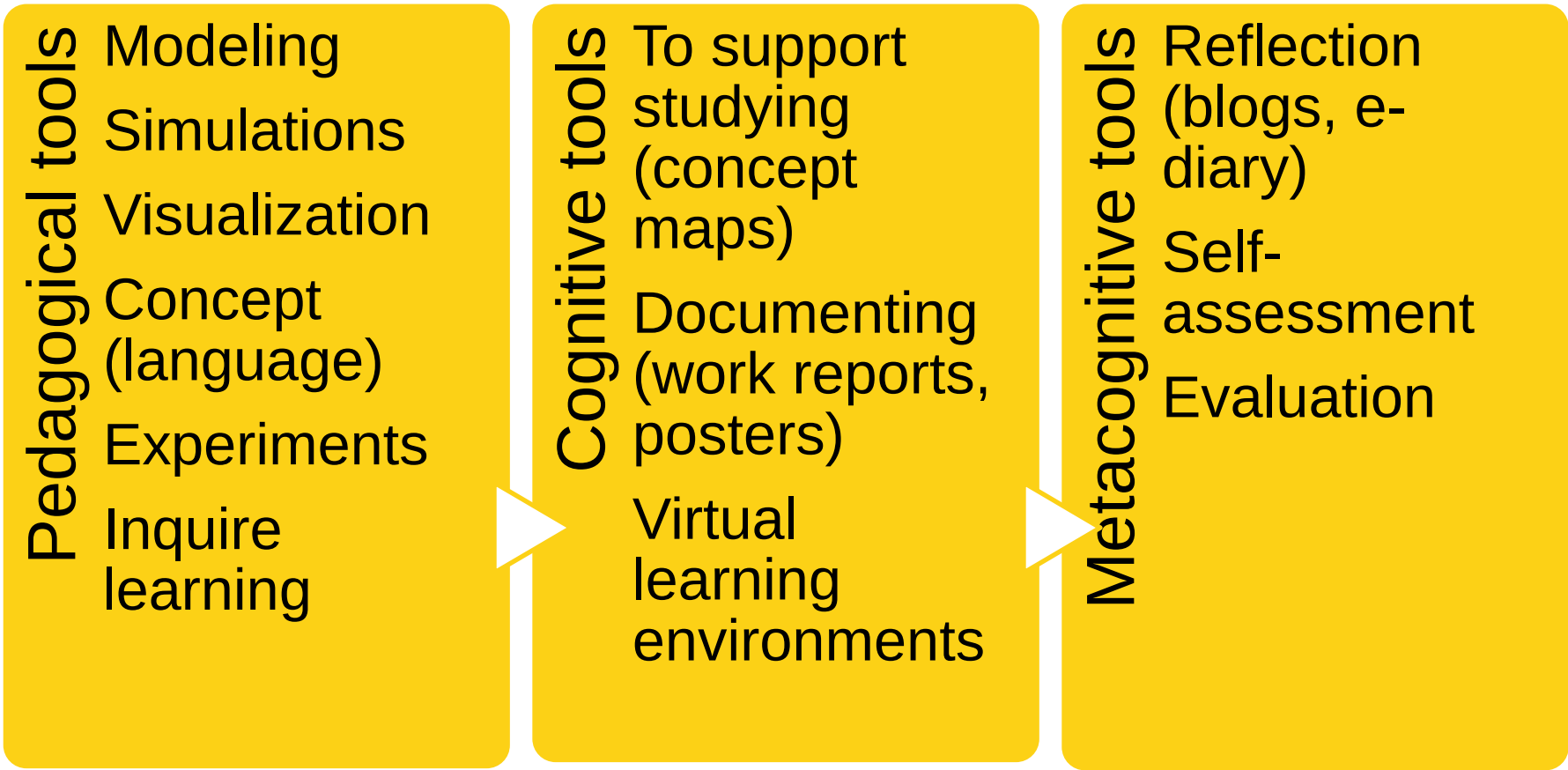
Fig. 2 An entangled pedagogy, including an aspirational view

Based on Shulman´s concept of Pedagogical Content Knowledge: TechPCK

- Are the ICT skills part of TechPCK or should we understand them in wider context



The whole picture of education (specially in science education)

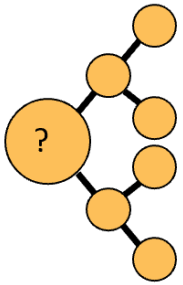


Nature of Science (chemistry)

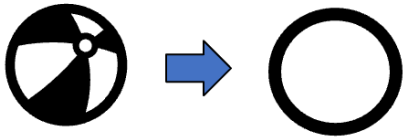
Shute (2017) has defined six approaches or processes within the CT concept or to describe how the CT concept can be applied

1. specification or decomposition, the whole consists of parts;
2. generalization or abstraction;
3. algorithmic thinking, design of algorithms;
4. data compaction, data collection and analysis, finding and modeling patterns;
5. efficiency;
6. debugging. These processes should iterative and transferable to new situations.

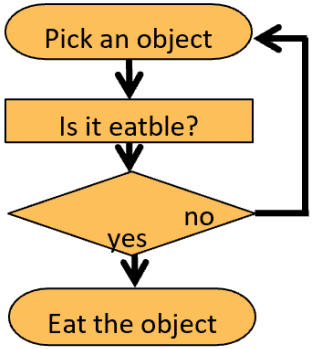
Cards based on Shute (2017)



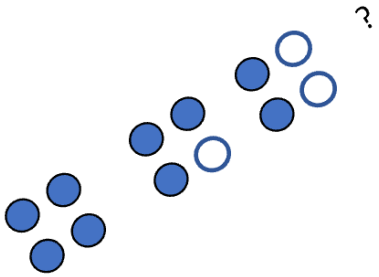
Decomposition: Dissect a complex problem/system into manageable parts.



Abstraction: Simplyfying an object or procedure



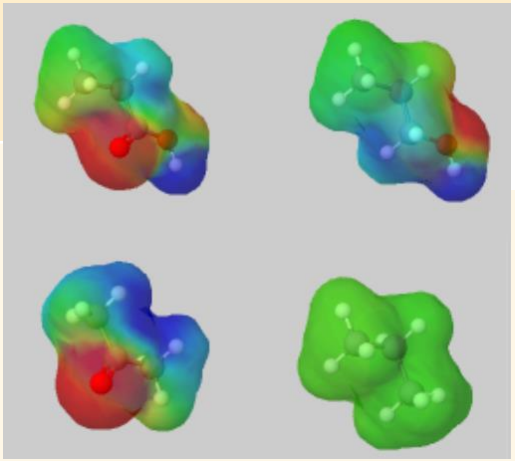
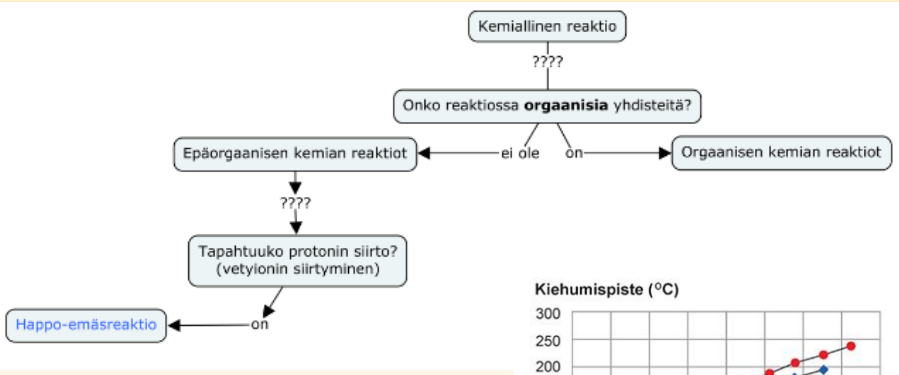
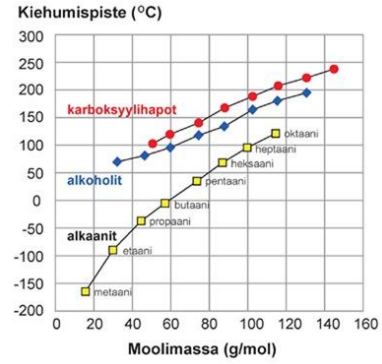
Algorithm: working according to an algorithm



Pattern recognition: Identify patterns/rules underlying the data/information structure

Efficiency: Design the fewest number of steps to solve a problem

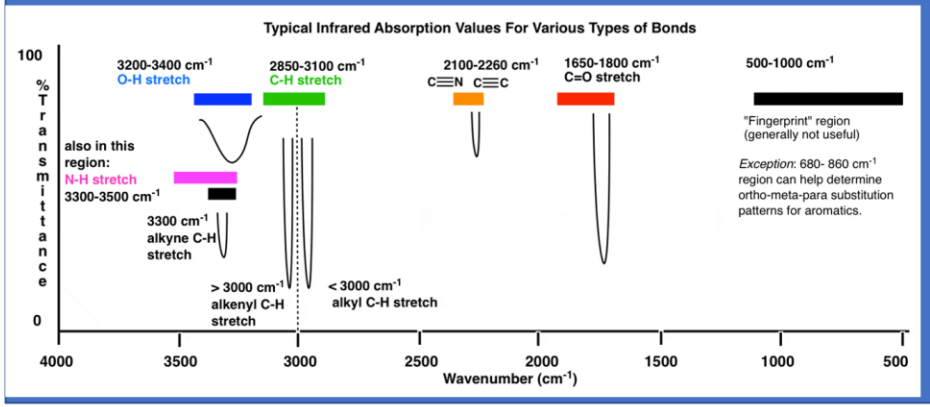
Debugging: evaluating behaviour of an object, procedure

Shute:	In concrete
Decomposition	**Chemical reactions – What kind of different parts these different chemical reactions include?**
Abstraction	**Spectroscopy analysis**
Algorithms	 
Patterns	
Efficiency	Finding tools to make things easier, faster, logical, using programing
Debugging	Creating own models, algorithms – testing – improve (next version)

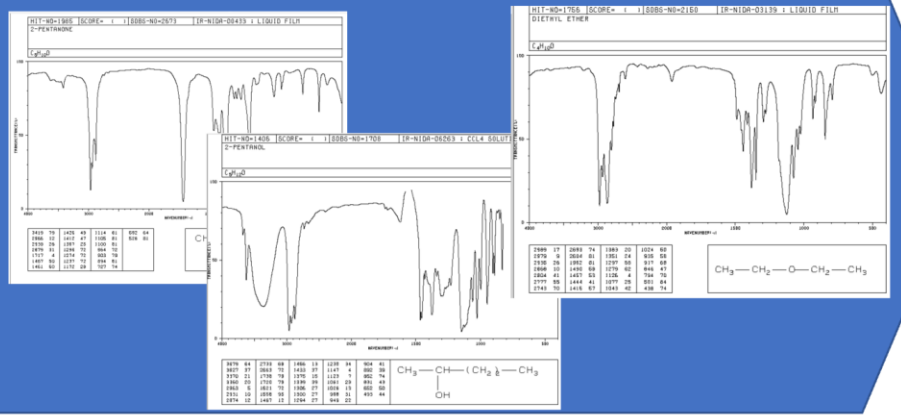
Teaching Spectroscopy?

Traditional

Spectral library (ready made)

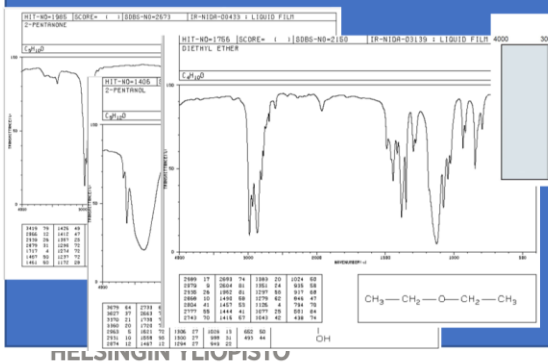


Spectral interpretation



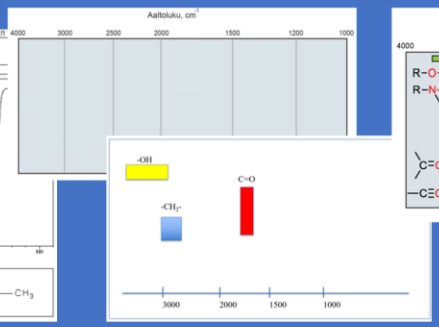
Modeling – Algorithmic thinking

Spectral interpretation
Spectral database

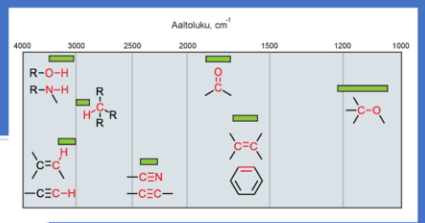


Scientific Practice - Modeling

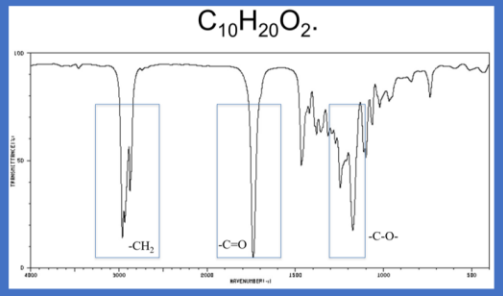
Spectral library (own)



Spectral library (group)



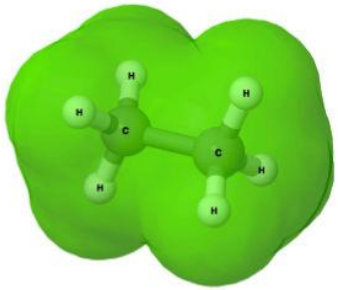
Spectral library (testing)



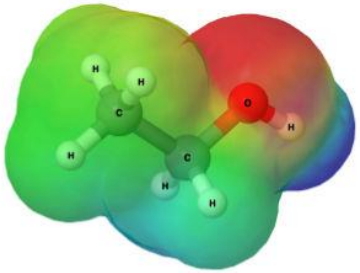
Algoritmic process in analysing chemical reaction

Working paper

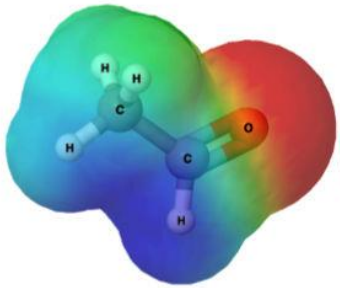
Using 3D-modeling programs – Electronegativity? Pattern!



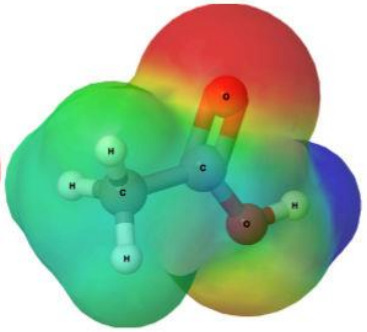
Ethane



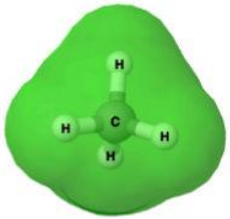
Ethanol



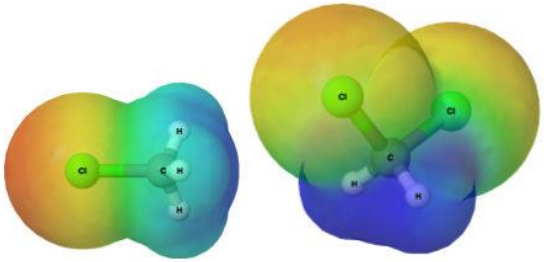
Ethanal



Ethan acid



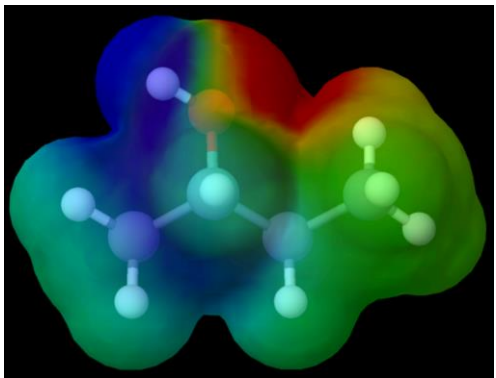
Methane



Tetracloromethane

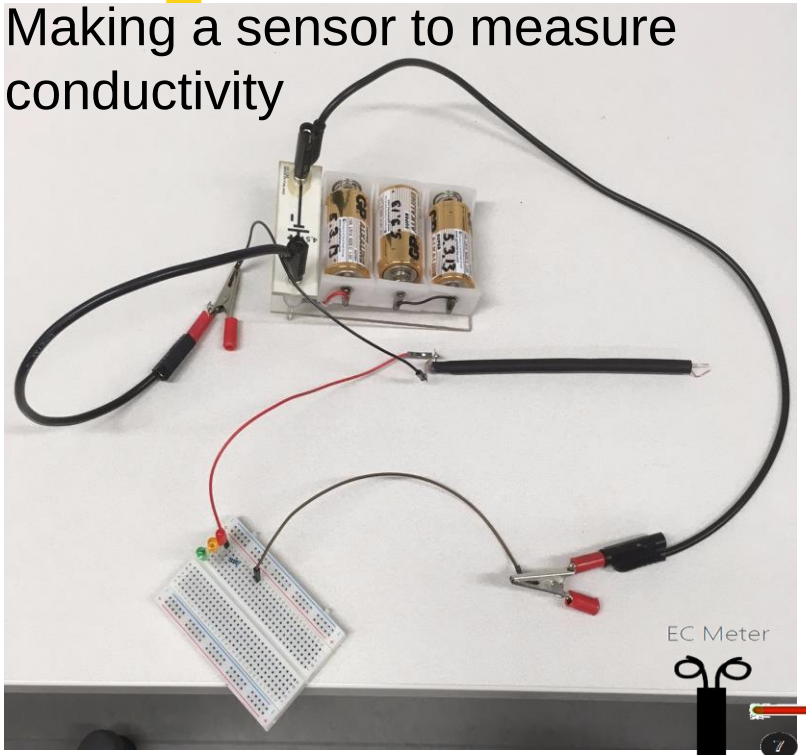
Concepts:

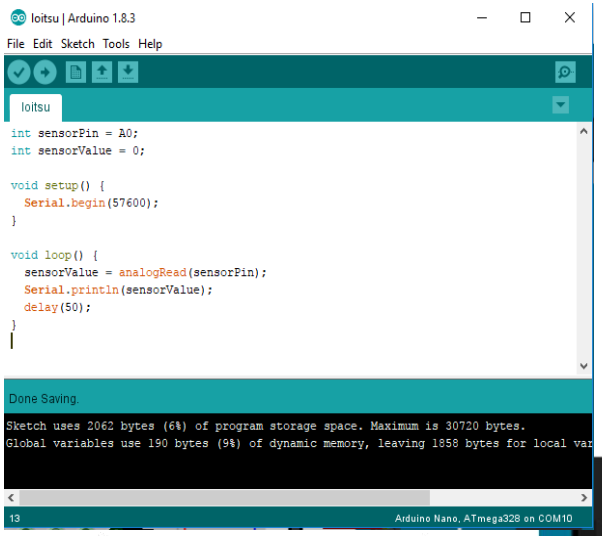
- Electron density
- Electronegativity
- Polar molecules
- Weak bonds

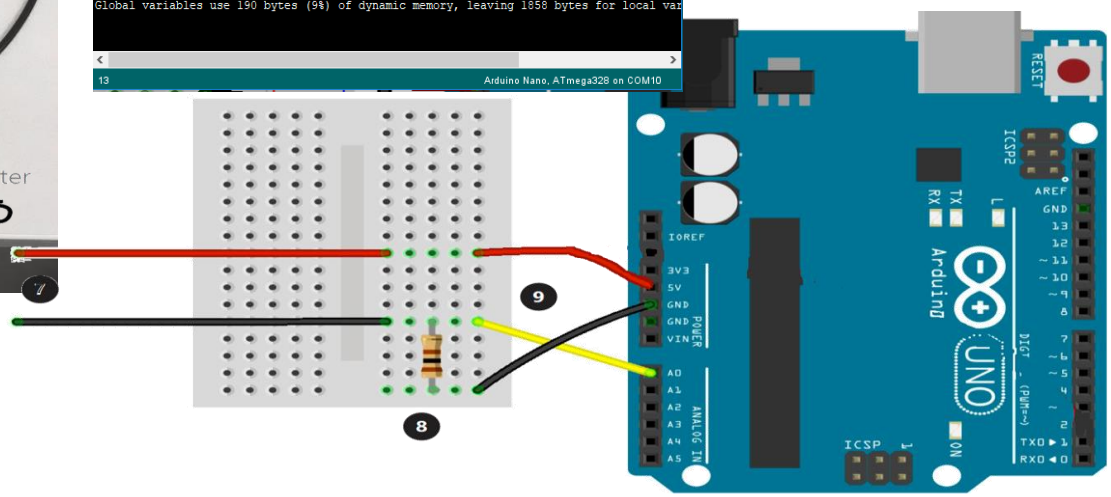


Idea about having programming in chemistry education

Making a sensor to measure conductivity







Writing a program for Arduino to measure conductivity