

Development of a Simulator for Explaining Organic Chemical Reactions Based on Qualitative Process Theory

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Abstract—This paper discusses the development of a qualitative simulator (abbreviated QRiOM) for predicting the behaviour of organic chemical reactions. The simulation technique is based on the qualitative process theory (QPT) ontology. The modelling constructs of QPT embody notions of causality which can be used to explain the behaviour of a chemical system. The major theme of this work is that, in a qualitative simulation environment, students are able to articulate his/her knowledge through the inspection of explanations generated by software. The implementation languages are Java and Prolog. The software produces explanation in various forms that stresses on the causal theories in the chemical system which can be effectively used to support learning.

Keywords—Chemical reactions, explanation, qualitative process theory, simulation

I. INTRODUCTION

In organic chemical reactions, one has to understand the many cognitive steps (the “mechanisms”) involved before a stable product is formed. Understanding these cognitive steps is among the many difficulties faced by chemistry students. Traditional chemistry educational software is inadequate in promoting understanding such as why and how things happen. These programs do not “explain” simply because the results are obtained through chaining of rules or by searching the reaction routes that have been pre-coded in software. Consequently, some students, particularly weak learners would require additional learning aids such as a software tool to assist them in their learning. In conventional approach, reaction prediction is performed by finding a route through searching the entire state space. Explanation generation is also a great challenge to this type of programming paradigm. Traditional chemistry software is therefore inadequate to promote understanding or explain toward its results because traditional method does not link “reasoning” to problems. This paper describes the development of a qualitative simulator for the simulation of organic chemical reactions. The simulator is based on the qualitative reasoning framework described in [1]. QRiOM (Qualitative Reasoning in Organic Mechanism) is the

product of the implementation of the framework. Qualitative process theory (QPT) [2] is used for the representation of chemical theories and chemical facts. QPT is well-known ontology for qualitative reasoning (QR). The development of QRiOM was motivated by a number of QR related systems reported in [3]-[11].

II. PREVIOUS WORK

This work combines qualitative reasoning and ontologies in a simulation system, and generates explanations for learners from the system. In [12], “make-bond” and “break-bond” chemical bonding have been identified as two generic processes in the simulation of organic chemical reactions. From the analysis of various chemical reactions occurring under S_N1 and S_N2 mechanisms, the common set of chemical theories and behaviour for the generic processes have been identified, from which the model automation procedures are formulated. A set of QR algorithms used for the simulation of reactions have also been developed. The algorithms can cater for “select and sequence” ability, with the aid of the OntoRM ontology [13]. This paper will provide a few simulation results that serve as “explanation” to chemical phenomena related to organic reactions. Our approach for answer justification is based on causal reasoning. Overall, the issue of lack of explanation in chemistry software is addressed by embedding a causal explanation generator that produces explanation in various forms.

III. SOFTWARE ARCHITECTURE OF QRiOM

Fig. 1 depicts the software modules implemented in QRiOM. Table 1 describes the role of the main modules in the simulator. The knowledge-base has a two layer structure. The purpose of the lower layer is to provide chemical facts to the simulator. This layer is called chemical instances (or basic facts). Instances refer to chemical elements and their chemical properties that do not change over time. The upper layer is the chemistry ontology for reaction mechanisms simulation. This tier is called OntoRM. The ontology defines the requirements and constraints when suggesting a reaction mechanism for a chemical equation simulation.

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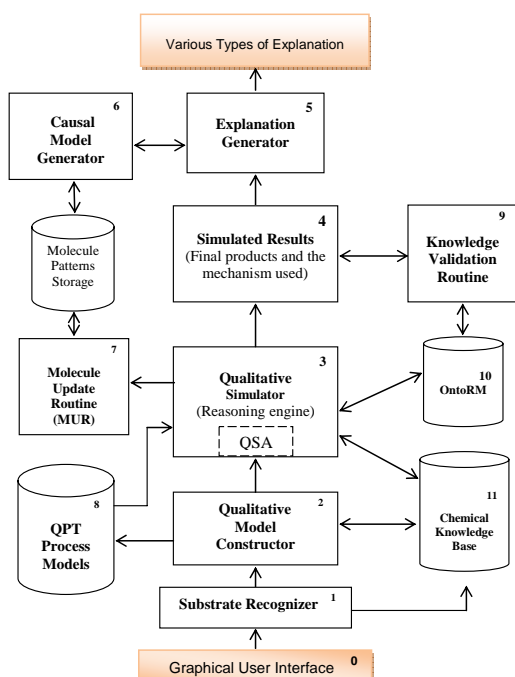
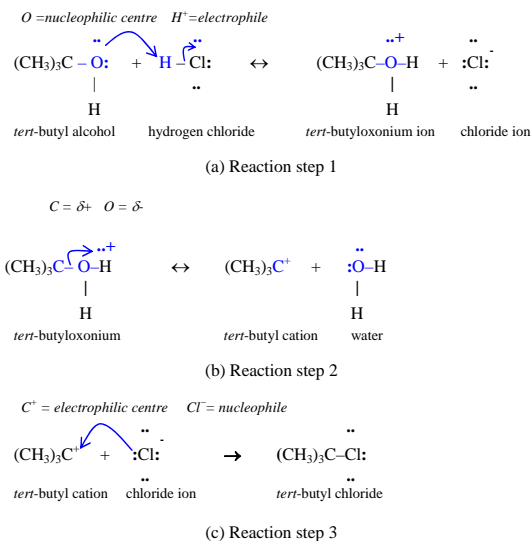


Fig. 1 Main software modules in QRiOM simulator

TABLE I
ROLES OF EACH MODULE IN QRiOM

Module	Roles
Module 1	This module checks user selection and returns the "type" of the input as either a nucleophile or an electrophile. From here on, an organic process may be determined.
Module 2	This module automates the construction of QPT models based on the identity of user inputs.
Module 3	This module does the actual reasoning and final product prediction.
Module 5	This module generates explanation on-the-fly based on causal reasoning.
Module 6	This module constructs causal graphs.
Module 7	This module keeps track of the structural change (pattern) of the substrate, from one organic reaction to another.
Module 9	The module validates the use of data <i>during</i> (to ensure the right data is passed to the reasoning engine) and <i>after</i> a simulation is completed (to ensure the results are predicted correctly).
Module 10	The reaction mechanism ontology that defines the basic chemical knowledge and chemical commonsense for S_N1 and S_N2 .

The chemical equation " $(CH_3)_3C-OH + HCl \rightarrow (CH_3)_3C-Cl + H_2O$ " will be used as the illustration example. The "thought processes" for the chemical equation is depicted in Fig. 2. It is necessary to build process models to describe the "thought" before reasoning or simulation can be initiated. Fig. 3 shows a process model represented in QPT. The QPT model can be used to reproduce the behaviour of the first reaction step for the " $(CH_3)_3C-OH + HCl$ " reaction (refer to part (a) of Fig. 2). Fig. 4 shows the simulation algorithm implemented in QRiOM.



Name of the chemical process	Reactant 1	Reactant 2
Protonation (= "make-bond")	$(CH_3)_3COH$ (nucleophile)	H^+ (electrophile)
Dissociation	$(CH_3)_3C-OH_2^+$	
Capturing of anion by carbocation	$(CH_3)_3C^+$ (electrophile)	Cl^- (nucleophile)

(d) Reactants and their associated chemical processes

Fig. 2 The conversion of a tertiary alcohol to yield alkyl chloride can be described as a series of three small steps

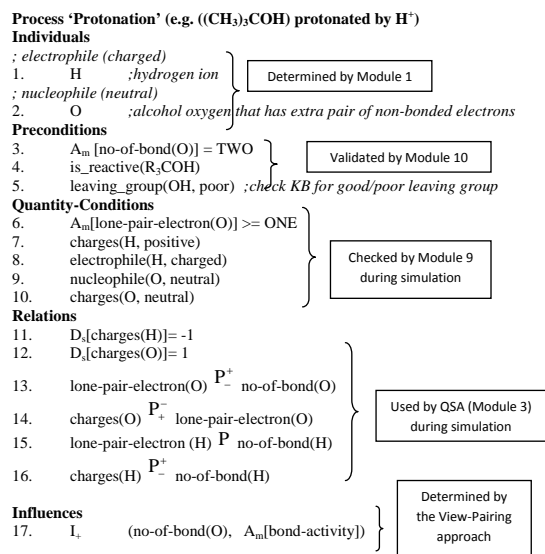


Fig. 3 QPT model for the "make-bond" process that links the proton to the oxygen atom in the tertiary alcohol substrate

QPT-BASED SIMULATION ALGORITHM

Q_Simulation(QPT_model, OUTPUT)

1. Perform qualitative reasoning on the constructed QPT model
 - 1.1 Store the process's entry conditions
 - 1.2 Store the directly influenced process quantity
 - 1.3 Keep track of the state transition (handled by the QSA module)
2. IF process_stopping_condition = true THEN
 - Store propagated effects in special purpose data structures
 - Store new individuals in the VIS
 - Update the VIS
 END_IF
3. Update the substrate's molecular structure (handled by the MUR module)
4. IF VIS contains reactive individuals THEN
 - Determine a suitable chemical process
 - Go to step 1
 ELSE
 - Retrieve final product from the VIS
 - Call OntoRM to check for validity of the predicted product
 - Call OntoRM to check for the possible order of process execution
 - Write the final product and the proposed mechanism to OUTPUT
 END_IF
5. Return OUTPUT

Fig. 4 The QPT-based simulation algorithm for chemical process reasoning

IV. PROTOTYPE DEVELOPMENT

Fig. 5 shows the problem solving model of QRiOM (i.e. the protocol to interact with the software tool) while Fig. 6 gives the main interface of the qualitative simulator. QRiOM development is fully event-driven and object-oriented.

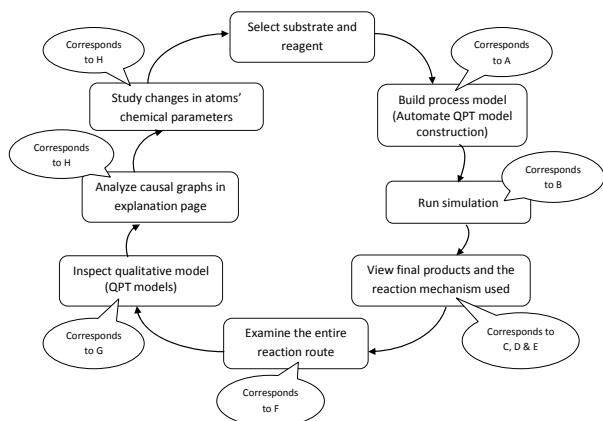


Fig. 5 Problem solving model (Labels A – H are in Fig. 6)

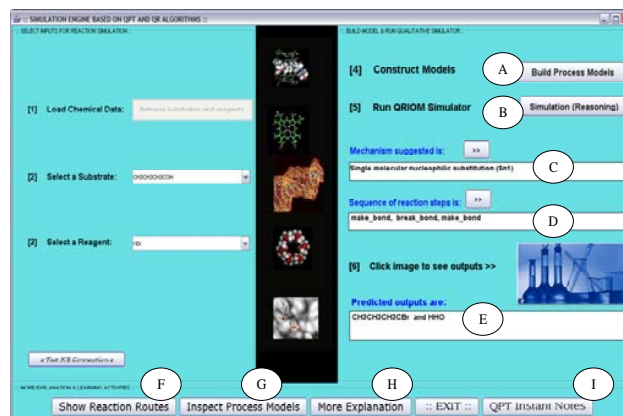


Fig. 6 The main interface of the simulator prototype

Apart from the final products, the simulator will produce the following results to explicate a phenomenon being asked: (1) qualitative model for organic processes, (2) view pairs used in the simulation, (3) causal graphs, (4) parameter state history for each atom that is involved in a reaction, and (5) overall structural change of the substrate. All of which are derived from the process model directly. As shall be shown, describing the domain knowledge in qualitative terms (via the modelling constructs of QPT) is sufficient to explain organic chemical phenomena. The following subsections present a few simulation outcomes (QPT model, view pairs, and causal graph) and the Java code for implementing them.

A. Java Snippets for the Construction of QPT Models

QPT model serves the educational objective of "knowledge articulation" of various aspects of a chemical reaction. When inspecting a QPT process model, students have to articulate relationships between entities and dependencies. Fig. 7 shows the Java code that retrieves the chemical facts from the chemical KB in order to construct a QPT model while a screenshot of model inspection page is shown in Fig. 8.

```

public void viewModel_actionPerformed(ActionEvent e) {
    amzi.ls.LogicServer ls = new amzi.ls.LogicServer();
    :
    String pn = gd.ProName;
    String ind1 = gd.View1;
    String ind1Type = gd.Type1;
    String ind2Type = gd.Type2;
    String ind2 = gd.View2;
    :
    JTextArea2.setFont(new java.awt.Font("Dialog", Font.BOLD, 12));
    JTextArea2.append("Process Activated: " + gd.ProNameList[0] + "\n");
    JTextArea2.append("\n" + "Individuals (The reacting units in this process/step)" + "\n");
    JTextArea2.setFont(new java.awt.Font("Dialog", Font.PLAIN, 10));
    JTextArea2.append(" " + gd.ViewList1_sn2[0] + " " + gd.ViewList2_sn2[0] + "\n");
    JTextArea2.setFont(new java.awt.Font("Dialog", Font.BOLD, 12));
    JTextArea2.append("\n" + "Quantity-Condition (Entry requirements to activate the process)" + "\n");
    JTextArea2.setFont(new java.awt.Font("Dialog", Font.PLAIN, 10));
    :
    ls.Load("bondKB.xml");
    term1 = ls.CallStr("qty_cond"+"gd.ProNameList[0]+", "gd.TypeList1[0]+", X, Y, Z, ");
    do
    {
        JTextArea2.append(" " + ls.GetStrArg(term1, 3) + " (" + ls.GetStrArg(term1, 4) + ") " +
            ls.GetStrArg(term1, 5) + "\n");
    } while (ls.Redo());
    term2 = ls.CallStr("qty_cond"+"gd.ProNameList[0]+", "gd.TypeList2[0]+", X, Y, Z, ");
    do{
        JTextArea2.append(" " + ls.GetStrArg(term2, 3) + " (" + ls.GetStrArg(term2, 4) + ") " +
            ls.GetStrArg(term2, 5) + "\n");
    } while (ls.Redo());
    :
    JTextArea2.setFont(new java.awt.Font("Dialog", Font.BOLD, 12));
    JTextArea2.append("\n" + "Influences (Direct effect caused by the process)" + "\n");
    JTextArea2.setFont(new java.awt.Font("Dialog", Font.PLAIN, 10));
    if (gd.ProNameList[0].equals("make_bond"))
    {
        JTextArea2.append(" " + "A covalent bond is added (formed)" + "\n");
    } else {
        JTextArea2.append(" " + "A covalent bond is removed (cleaved)" + "\n");
    }
    :
    JTextArea2.setFont(new java.awt.Font("Dialog", Font.BOLD, 12));
    JTextArea2.append("\n" + "Parameters dependency (Effects propagation)");
    JTextArea2.setFont(new java.awt.Font("Dialog", Font.PLAIN, 10));
    do{
        JTextArea2.append(" " + ls.GetStrArg(term3, 3) + " (" + ls.GetStrArg(term3, 5) + ") followed
            ls.GetStrArg(term3, 4) + " (" + ls.GetStrArg(term3, 6) + ") " + "\n");
    } while (ls.Redo());
    :
    JTextArea2.append("\n" + gd.ViewList2[0] + " [" + gd.TypeList2[0] + "]" + ":" + "\n");
    term3 = ls.CallStr("process_relations(make_bond, "+gd.TypeList2[0]+", P, Q, R, S, ");
    do{
        JTextArea2.append(" " + ls.GetStrArg(term3, 3) + " (" + ls.GetStrArg(term3, 5) + ") followed
            ls.GetStrArg(term3, 4) + " (" + ls.GetStrArg(term3, 6) + ") " + "\n");
    } while (ls.Redo());
    :
}

```

Prepare the individuals for the chemical process

Based on the view's type, general set of chemical theories are retrieved from the KB

Prepare the headings for the QPT model, and the direct influence of the process

Display the effect propagation caused by the process. These are the indirect influences of a QPT model

Fig. 7 The Java code for retrieving chemical theories of reacting species for constructing QPT model

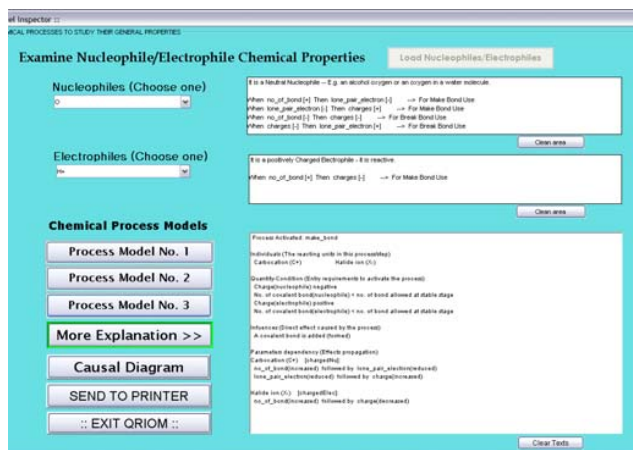


Fig. 8 The QPT model inspection page of QRiOM

B. Java Snippets for Implementing the Reasoning Engine

Quantity Space Analyzer (QSA) is one the important software modules in QRiOM. This module performs tasks such as updating and maintaining multiple data structures whenever an organic process is activated. Since the majority of chemistry students have difficulties identifying the right reacting units for processes activation, the tool will generate the whole set of reacting units (called "view pairs" in QPT)

used in the entire simulation thus informing the learner of the types of reacting species that activated a given chemical process (Fig. 9). The Java code for "view structure updating" is presented in Fig. 10. These results can then be used to generate the necessary reaction route for the entire simulation of a chemical equation.

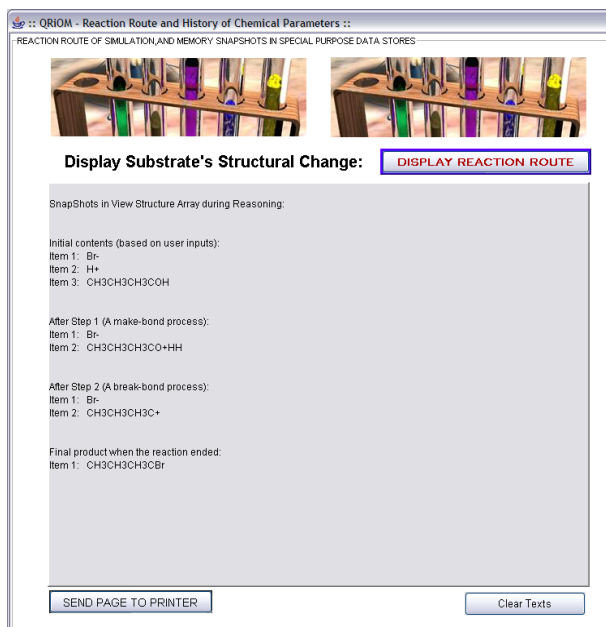


Fig. 9 The choice of reacting units for each reaction step and the intermediates produced are displayed for further inspection

```

:
if (Subst_1_ChargedHistory[4].equals("pos"))
{
    appendedCharge1 = StartMaterialTable[0].concat("+"); // Check its charge's state
    theStr1 = "CH3CH3CH3".concat(appendedCharge1);
} else if (Subst_1_ChargedHistory[4].equals("neg"))
{
    appendedCharge1 = StartMaterialTable[0].concat("-");
    theStr1 = "CH3CH3CH3".concat(appendedCharge1);
} else theStr1 = "CH3CH3CH3".concat(StartMaterialTable[0]);

if (Agent_2_ChargedHistory[4].equals("pos"))
{
    appendedCharge1 = StartMaterialTable[1].concat("+");
    theStr2 = theStr1.concat(appendedCharge1);
} else if (Agent_2_ChargedHistory[4].equals("neg"))
{
    appendedCharge1 = StartMaterialTable[1].concat("-");
    theStr2 = theStr1.concat(appendedCharge1);
} else theStr2 = theStr1.concat(StartMaterialTable[1]);

```

ViewStructureArr[0] = theStr2; // Update the contents of VIS

Fig. 10 The Java statements for updating the VIS in order to suggest the next organic process in the qualitative simulation environment

Fig. 11 gives the Java snippets for updating changes in parameters' states. The values assigned to the chemical parameters during simulation are recorded in special purpose data structures for future retrieval. One such structure is the atom property table (Fig. 12).

```

ls.Init("");
ls.Load("chemkb.xml");

t1 = ls.CallStr("qpropAPTable(make_bond, chargedElec, P3, Q3, R3, S3); // Prepare to retrieve chemical theories
if (t1 == 0)
{
    ls.Close();
    return;
}

do{
    if (n1 == 1){
        qtyArrTemp[0] = ls.GetStrArg(1, 3);   qtyArrTemp[1] = ls.GetStrArg(1, 4);
        signArrTemp[0] = ls.GetStrArg(1, 5);   signArrTemp[1] = ls.GetStrArg(1, 6);
    }
    if (n1 == 2){
        qtyArrTemp[2] = ls.GetStrArg(1, 3);   qtyArrTemp[3] = ls.GetStrArg(1, 4);
        signArrTemp[2] = ls.GetStrArg(1, 5);   signArrTemp[3] = ls.GetStrArg(1, 6);
        n1++;
    } while (!s.Redo());
}

if ((individual_2_type.equals("chargedElec") && (bActivity.equals("make_bond")))
    {
    if ((signArrTemp[0].equals("plus") && (qtyArrTemp[0].equals("charge")))
        {
        for (int t=0; t<=2; t++)
        {
        if (charge[t].equals(smt_0_ChargeVal) index = t;
            gdat.Sub_1_ChargedHistory[4] = Subst_1_ChargedHistory[4]
            = charge[t].equals("minus") ? Subst_1_ChargedHistory[4] - 1 :
            charge[t].equals("plus") ? Subst_1_ChargedHistory[4] + 1 :
            charge[t];
            if (charge[t].equals(smt_0_ChargeVal) index = t;
                gdat.Sub_1_ChargedHistory[4] = Subst_1_ChargedHistory[4] = charge[t].equals("minus") ?
                Subst_1_ChargedHistory[4] - 1 : charge[t].equals("plus") ? Subst_1_ChargedHistory[4] + 1 :
                charge[t];
            }
        }

    if ((signArrTemp[0].equals("plus") && (qtyArrTemp[0].equals("lone_pair_electron")))
        {
        for (int t=0; t<=4; t++)
        {
        if (String.valueOf(lone_pair[t]).equals(smt_0_LPVal) index = t;
            gdat.Sub_1_LonePairHistory[4] = Subst_1_LonePairHistory[4] =
            String.valueOf(lone_pair[t].equals("minus") ? Subst_1_LonePairHistory[4] - 1 :
            lone_pair[t].equals("plus") ? Subst_1_LonePairHistory[4] + 1 : lone_pair[t]);
            if (String.valueOf(lone_pair[t]).equals(smt_0_LPVal) index = t;
                gdat.Sub_1_LonePairHistory[4] = Subst_1_LonePairHistory[4] =
                String.valueOf(lone_pair[t].equals("minus") ? Subst_1_LonePairHistory[4] - 1 :
                lone_pair[t].equals("plus") ? Subst_1_LonePairHistory[4] + 1 : lone_pair[t]);
            }
        }

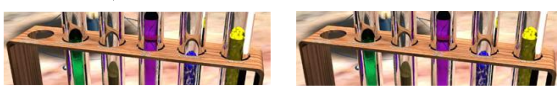
    if ((signArrTemp[0].equals("plus") && (qtyArrTemp[0].equals("no_of_bond")))
        {
        for (int t=0; t<=4; t++)
        {
        if (String.valueOf(bond[t]).equals(smt_0_BondVal) index = t;
            gdat.Sub_2_BondHistory[4] = Subst_2_BondHistory[4] = String.valueOf(bond[t].equals("minus") ?
            Subst_2_BondHistory[4] - 1 : bond[t].equals("plus") ? Subst_2_BondHistory[4] + 1 : bond[t]);
            if (String.valueOf(bond[t]).equals(smt_0_BondVal) index = t;
                gdat.Sub_2_BondHistory[4] = Subst_2_BondHistory[4] = String.valueOf(bond[t].equals("minus") ?
                Subst_2_BondHistory[4] - 1 : bond[t].equals("plus") ? Subst_2_BondHistory[4] + 1 : bond[t]);
            }
        }
    }
}

```

Fig. 11 The Java code for updating the chemical parameters' states of each atom during simulation

QRiOM - Reaction Route and History of Chemical Parameters

REACTION ROUTE OF SIMULATION AND MEMORY SNAPSHOTS IN SPECIAL PURPOSE DATA STORES



Display Substrate's Structural Change:

Substrate change during the 3-Step reaction, by the proposed mechanism: Sml

Initial atoms and their chemical states:

Name	Charge	No. of Bond	Lone Pair Electrons
C	neutral	4	0
O	neutral	2	2
H	neutral	1	0

After Step 1: a make-bond process:

Name	Charge	No. of Bond	Lone Pair Electrons
C	pos	3	1
H	neutral	1	0
H	neutral	1	0

After Step 2: a break-bond process:

Name	Charge	No. of Bond	Lone Pair Electrons
C	pos	3	0

After Step 3: a make-bond process:

Name	Charge	No. of Bond	Lone Pair Electrons
C	neutral	4	0
Br	neutral	1	3

Fig. 12 The chemical states possessed by each reacting unit during simulation are stored in atom property table

C. Java Snippets for Causal Graph Generator

Algorithms determine what the behaviour is, not an explanation of it. An explanation of system behaviour may

take many forms. An example is causal accounts (or causality). Causal account is a kind of explanation that is consistent with our intuitions of how systems function. The explanation used by QRiOM is achieved by tracing the cause-effect propagation through the modelling constructs of QPT. For example, during each reaction simulation, a causal graph (Fig. 13) is generated that shows the use of the qualitative proportionality statements (or functional dependency) in the QPT models. Fig. 14 shows the Java code that generates causal graphs for explaining the cause-effect interaction among all the parameters.

CAUSAL DIAGRAM INSPECTION

DIAGRAM SHOWING FUNCTIONAL DEPENDENCY OF PARAMETERS

This is the causal diagram for the reaction formula you just selected

Step 1: Break-Bond Process

Nucleophile(C)	Electrophile(Br)
no_of_bond(no change)	no_of_bond(minus)
charge(plus)	charge(minus)
	lone_pair_electron(plus)

CH3CH3CH3C+

Step 2: Make-Bond Process

Nucleophile(C+)	Electrophile(H2O)
charge(minus)	no_of_bond(plus)
no_of_bond(plus)	lone_pair_electron(minus)
lone_pair_electron(nil)	charge(plus)

CH3CH3CH3CO+H2 (Carbocation as intermediate)

Step 3: Break-Bond Process

Nucleophile(O+)	Electrophile(H)
no_of_bond(minus)	no_of_bond(minus)
lone_pair_electron(plus)	charge(plus)
charge(minus)	

CH3CH3CH3COH

Predicted product is : CH3CH3CH3COH

Fig. 13 A causal graph generated by QRiOM that enables learners to examine the cause-effect relationships of chemical parameters during reasoning

```

public void causalGraph_actionPerformed(ActionEvent e) {
    globalDataEG gd = new globalDataEG();

    jCG.setText("");
    jCG.append("\nThis is the causal diagram for the reaction formula you just selected\n");

    if (gd.procnInvolved[0].equals("make_bond")){
        jCG.append("Step 1: Make-Bond Process\n");
        jCG.append("Nucleophile" + "(" + gd.smn + ")" + "\n" + "Electrophile" + "(" + gd.aat00 + ")" + "\n");

        for(int y=0; y<=2; y++){
            if(!gd.par1[y].equals("nil"))
                if (y==1)
                    jCG.append("\n" + gd.par1[y] + "(" + gd.sign1[y] + ")" );
                else jCG.append("\n" + gd.par1[y] + "(" + gd.sign1[y] + ")" );
            else jCG.append("\n");
            if(!gd.par2[y].equals("no change"))
                if (y==2)
                    jCG.append("\n" + gd.par2[y] + "(" + "no change" + ")" + "\n");
                else if (y==1)
                    jCG.append("\n" + gd.par2[y] + "(" + gd.sign2[y] + ")" + "\n");
                else jCG.append("\n" + gd.par2[y] + "(" + gd.sign2[y] + ")" + "\n");
            else jCG.append("\n");
        }
    }
}
// End Generate Causal Graph

```

These codes prepare the values taken by each main parameter during the entire reasoning and simulation. The set of values are then formatted onto the appropriate user graphical interfaces

Fig. 14 The Java code that keeps track of the values assigned to each parameter during reasoning. The set of values will be retrieved and formatted to graphical user interface

When the outputs of causal graph, QPT model, and atom property table are examined together, the students are expected to relate various aspects in a reaction such that they are able to explain an organic reaction in a more elaborate way. This will lead to an improvement in one's conceptual understanding of the subject.

V. CONCLUSION

A qualitative simulation environment that enables students to articulate his/her knowledge through the inspection of explanations generated by software has been described. The implementation of the main modules in the reasoning engine has also been presented as a collection of Java snippets. QRiOM is the first chemistry education software that can generate multiple forms of textual explanation via QPT-based reasoning. QRiOM is viewed as useful and effective by chemistry learners, consistent with the fact that students' conceptual understanding is improved [14].

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