Comparison of Computer Simulation Methods for Predicting Chemical Reactions

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In this paper we compare two primary methods of predicting basic organic chemistry reaction predictions. We analyze two types of models, an NLP based Neural Network and an agent based model. We compare and contrast the complexity, accuracy, and generalizability of both models as applied to predicting organic chemistry reactions. Two basic reaction mechanisms are explored, Elimination and Addition reactions. These two mechanisms are simple but fundamental to the set of organic reactions, as many more complicated reactions use this mechanisms as intermediates. We first verify the model on an alkene halogen addition reaction and then investigate the models generalizability to the elimination reaction.

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I. INTRODUCTION

Using latex is pretty easy if you have a sample document you can follow.

II. RESULTS

Including figures, tables, and equations is easy. Latex also permits easy reference to document elements (figures, tables, sections) with the

`\ref`

command1. Citations are made with the

`\cite`

command[1].

FIG. 1: You will need to include the package graphicx to be able to make figures like this.

A simple table.

TABLE I: $X(3872)$ Discovery Modes.

mass	width	production/decay mode	events	significance	experiment
$3872.0 \pm 0.6 \pm 0.5$	< 2.3 90% C.L.	$B^{\pm} \to K^{\pm} X \to K^{\pm}\pi^{+}\pi^{-} J/\psi$	25.6 ± 6.8	10σ	Belle
$3871.3 \pm 0.7 \pm 0.4$	resolution	$p\bar{p} \to X \to \pi^{+}\pi^{-} J/\psi$	730 ± 90	11.6σ	CDFII
$M(J/\psi) + 774.9 \pm 3.1 \pm 3.0$	resolution	$p\bar{p} \to X \to \pi^{+}\pi^{-} J/\psi$	522 ± 100	5.2σ	DØ
3873.4 ± 1.4	–	$B^{-} \to K^{-} X \to K^{-}\pi^{+}\pi^{-} J/\psi$	25.4 ± 8.7	3.5σ	BaBar

And a sample equation (Eq. 1).

$$\Gamma(X \to \alpha\beta D) = \int \frac{d^3Q}{(2\pi)^3} \Gamma(C \to \alpha\beta) \frac{|\tilde{T}(Q)|^2}{(M(X) - E_{CD}(Q))^2 + \Gamma_C^2/4} \tag{1}$$

III. CONCLUSIONS

Man, latex is great!

Acknowledgments

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[1] *LaTeX : A Documentation Preparation System User's Guide and Reference Manual*, Leslie Lamport [1994] (ISBN: 0-201-52983-1) pages: xvi+272.
[2] I.M. Smart *et al.*, J. Plumb Phys. **50**, 393 (1983).