Appendix A

Manual for CRCP : Chemical Reaction Classifier and Predictor Software

This manual gives the steps or procedures required to follow so that user can properly use the software "CRCP : Chemical Reaction Classifier and Predictor". Through this manual user can learn how to input chemical reactions to generate templates and insert it into database, to delete reactions from database and also to predict products by giving inputs of chemical compounds. The user needs to open the software "CRCP : Chemical Reaction Classifier and Predictor". The opening screen will be as given in image in A.1

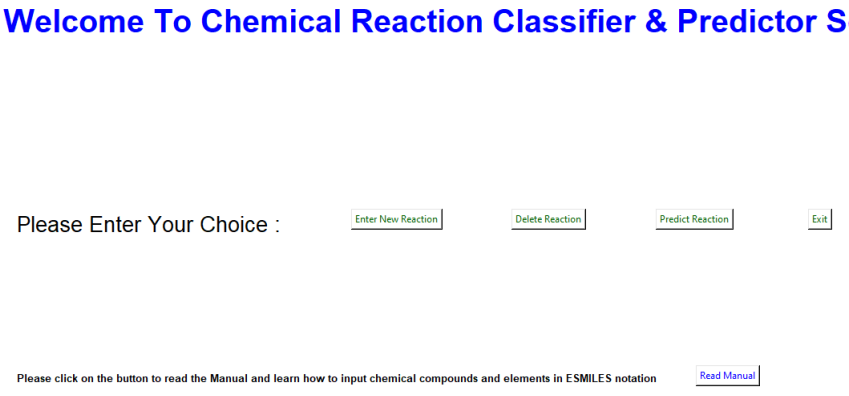

Figure A.1: Opening Screen of CRCP : Chemical Reaction Classifier and Predictor Software

The user needs to click on buttons given in image A.1 to enter, delete

or predict reactions. Sections 1, 2, 3 discusses about them respectively.

1 Procedure to enter new chemical reactions and generate templates

To enter new chemical reactions into the database and generate templates, the user needs to start the software and click on the button "Enter New Reaction". The screen appearing will be as shown in the image A.2.

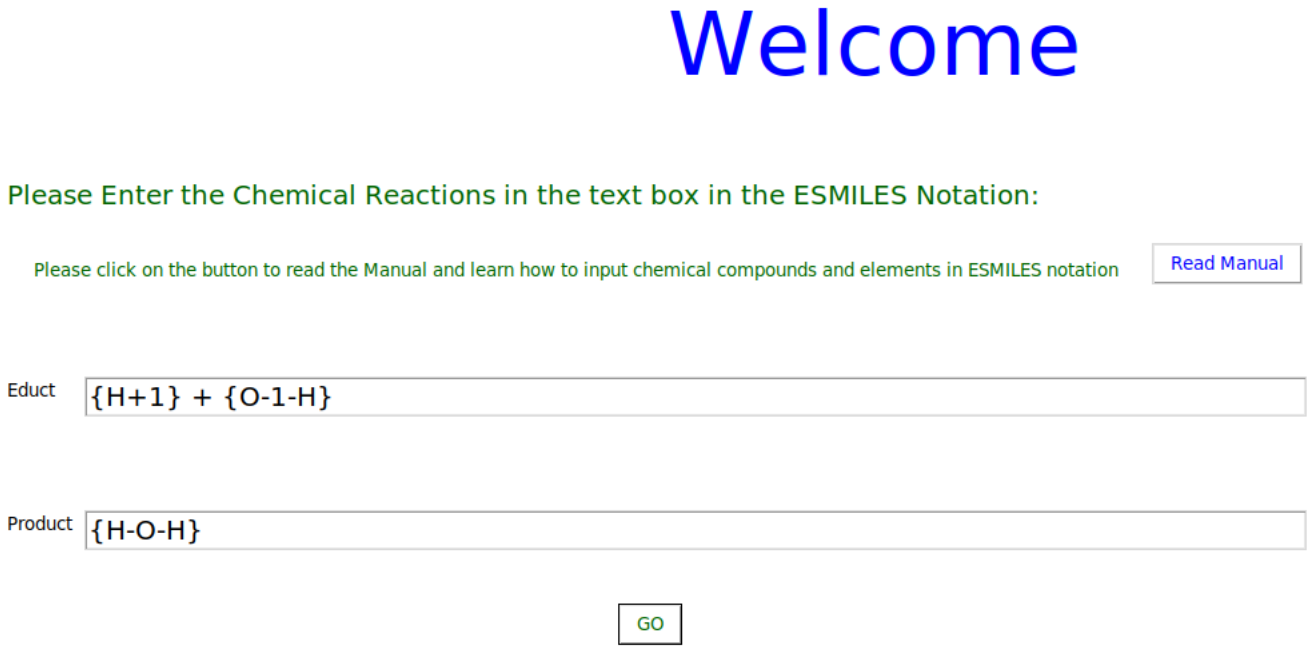

Figure A.2: Opening Screen with given inputs in ESMILES notation

The user needs to give the educts and products in the corresponding text boxes as shown in the image. The rule for giving chemical reaction inputs in ESMILES notation is provided in Appendix B. On clicking "Go" button the system will check if correct rules of ESMILES notation is given or not, if yes then the software will take the user to the the next screen which is given in image A.3.

Figure A.3: Screen to give serial number of product elements

The user needs to give serial number of each product element in the given space provided to specify the one on one correspondence between educt elements and product elements. After giving the serial numbers, the 'set' button is clicked. The next screen as shown in image A.4 gives the reaction and its corresponding templates. To store the reaction and templates into the database, the user needs to click "INSERT INTO DATABASE" button. On clicking the "REFERENCE" button, a new screen will appear as shown in image A.5, which gives the references for user to understand which symbol in template corresponds to which element in the reaction. The user should click on "EXIT" button to quit from the software.

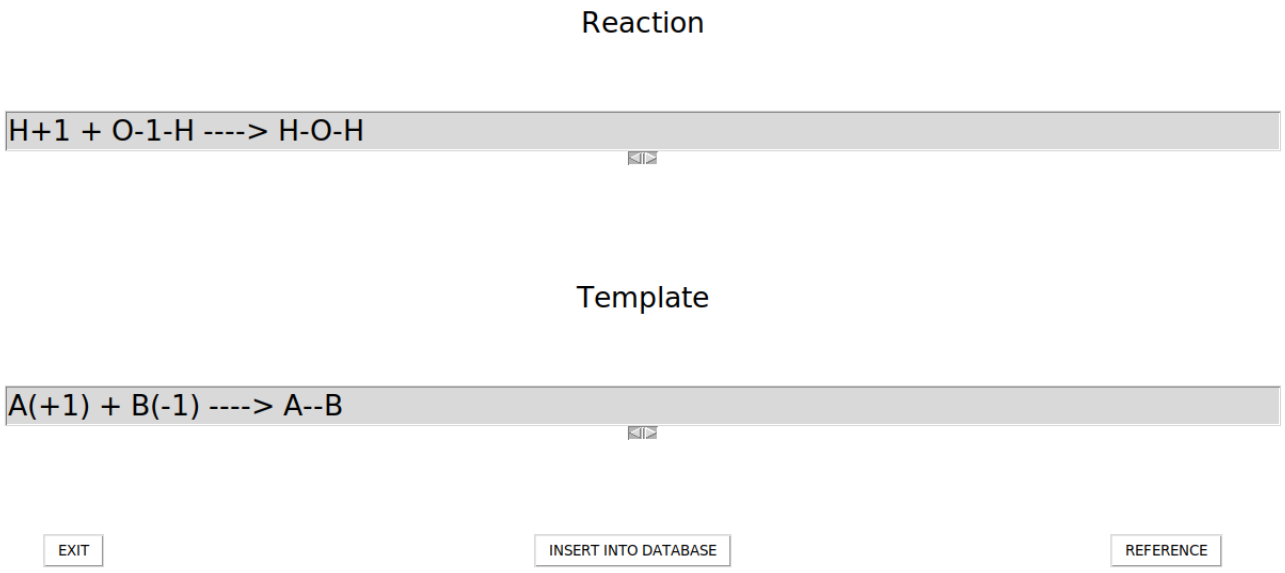

Figure A.4: Output Screen

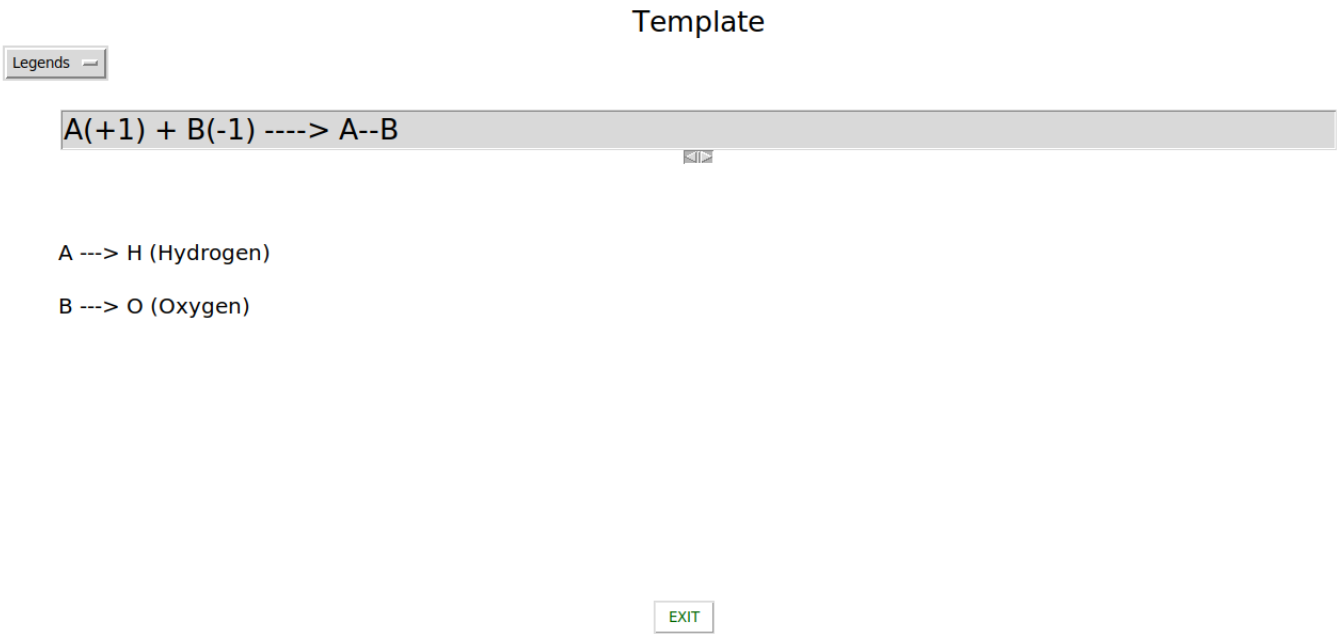

Figure A.5: Reference Screen

2 Procedure to delete chemical reactions from the data base

To delete chemical reactions from the database, the user needs to start the software and click on the button "Delete Reaction". The screen appearing will be as shown in the image A.6. The user needs to provide the educts and products in ESMILES notation B and then press on "delete" button. The software checks the ESMILES notation and then searches for the reaction in the database. If the reaction is found, it is deleted from the database as shown in image A.7.

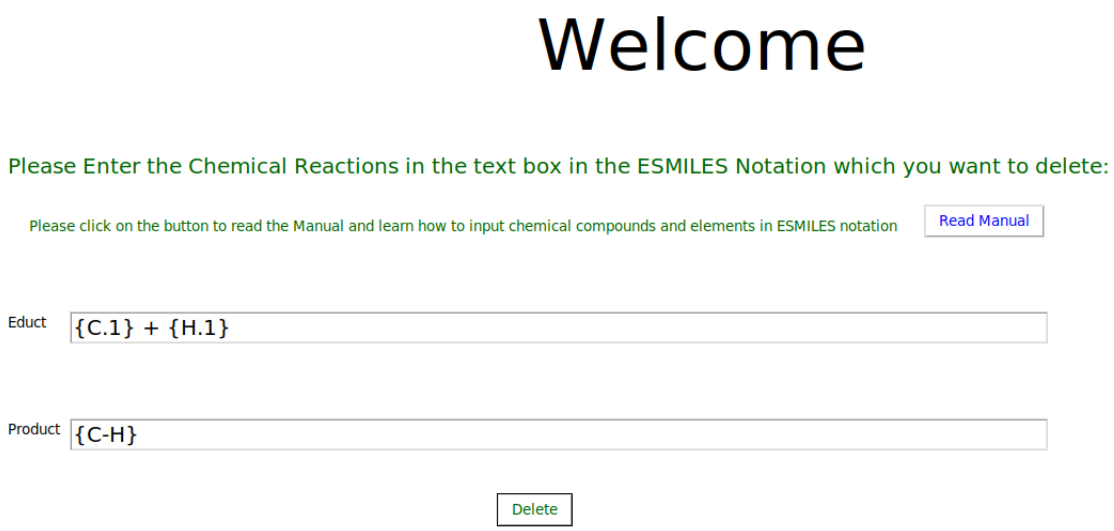

Figure A.6: Deletion Screen

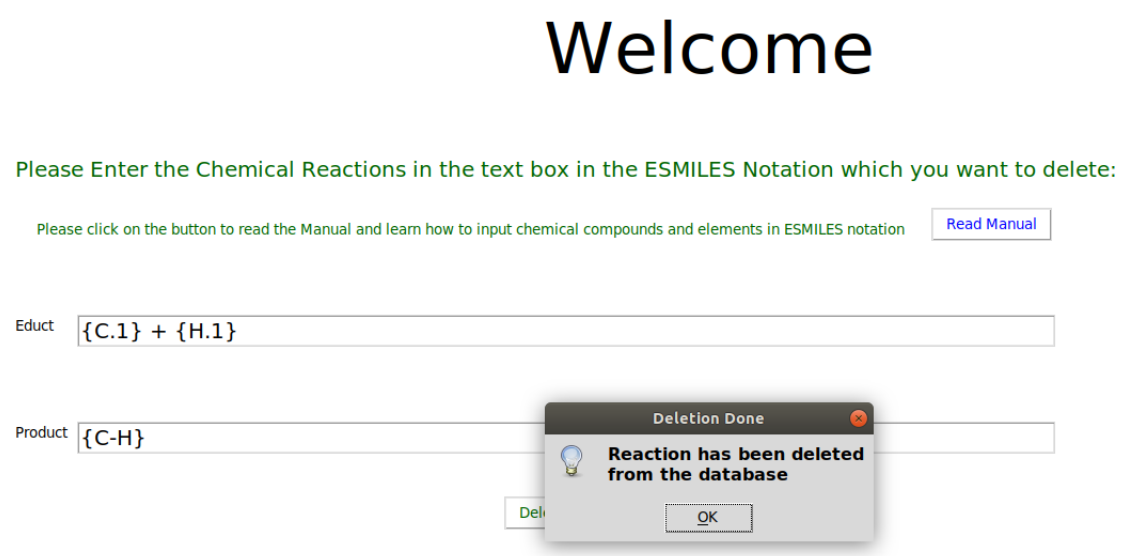

Figure A.7: Screen after deletion

3 Procedure to predict chemical reactions

To predict products of a chemical reaction by giving inputs of educts in ESMILES notation B, the user needs to click on the button "Predict Reaction" given in the screen in image A.1. On clicking the button, a screen will appear as shown in image A.8.

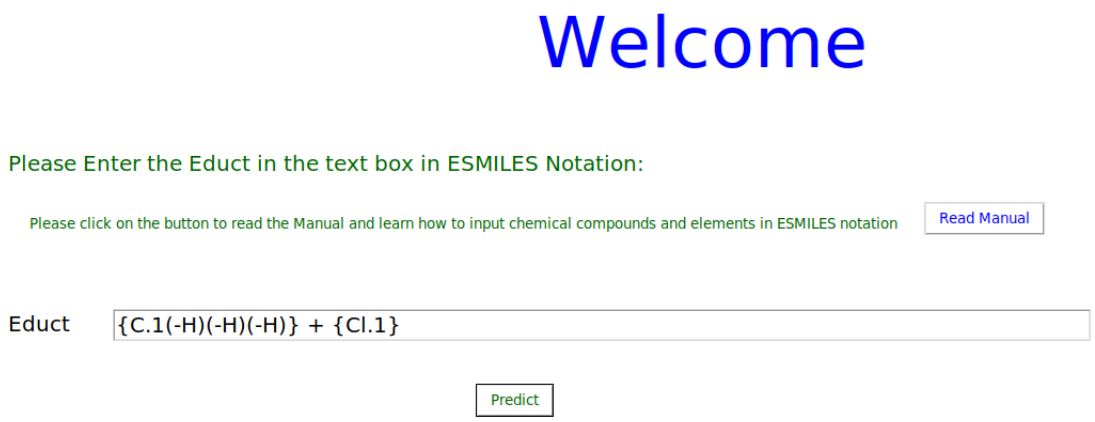

Figure A.8: Prediction Screen

The user needs to enter the ESMILES notation of the educt in the space provided and then click on the "Predict" button. The software checks whether the educt in ESMILES notation is valid or not. If valid, another screen will be displayed as shown in image A.9 which gives the list of products predicted.

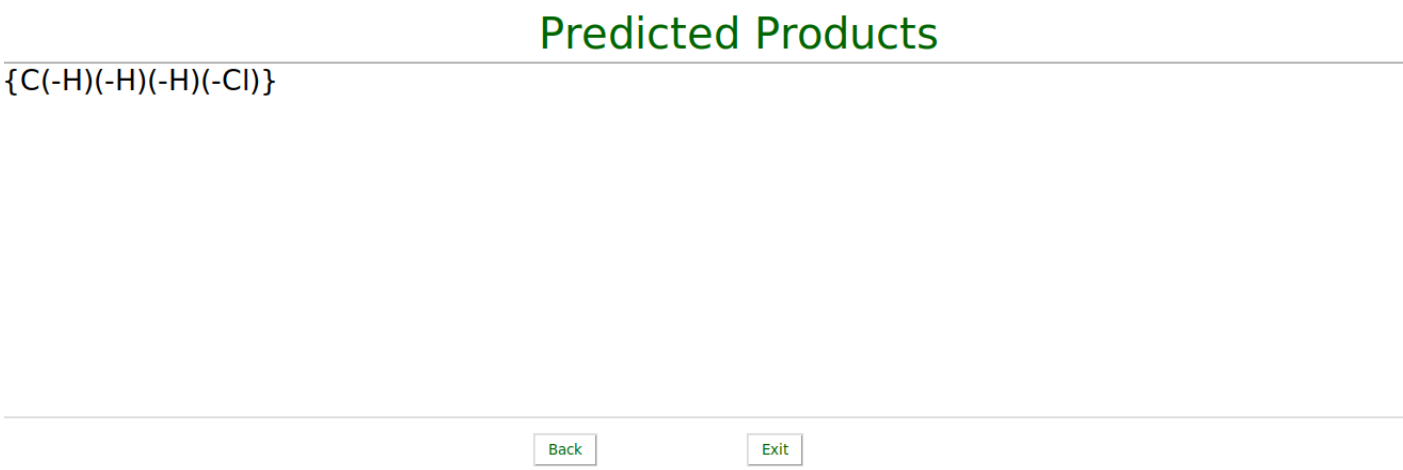

Figure A.9: List of Products