VISVESVARAYA TECHNOLOGICAL UNIVERSITY, BELAGAVI - 590018



Mini Project Report

On

"INORGANIC CHEMICAL REACTION PREDICTOR"

A report submitted in partial fulfillment of the requirements for

MINI PROJECT (21AIMP67)

In

Artificial Intelligence & Machine Learning

Submitted by

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Approved by AICTE, New Delhi, Recognized by Government of Karnataka.

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CERTIFICATE

This is to certify that the Mini Project entitled "INORGANIC CHEMICAL REACTION PREDICTOR" has been successfully completed by

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The Bonafide students of the Department of Artificial Intelligence and Machine Learning.

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TECHNOLOGICAL UNIVERSITY, BELAGAVI during the year 2023–2024. It is certified that all corrections/suggestions indicated for Internal Assessment have been incorporated in the report deposited in the departmental library. The Mini Project report has been approved as it satisfies the academic requirements in respect of the Mini Project work prescribed for the Bachelor of Engineering Degree.

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ABSTRACT

The goal of the Chemical Reaction Predictor project is to use machine learning methods to predict the results of chemical reactions. A model that forecasts the products created from given reactants can be developed by examining a sizable dataset of known reactions. This includes gathering and sanitizing data, identifying key characteristics such as reactant properties and reaction conditions, and creating several prediction models. The project's main goal is to implement algorithms like random forests and support vector machines and thoroughly train them to provide results with 66.67% accuracy. To ensure these models are effective, we assess them using measures like accuracy, precision, recall, and F1 score. After determining the optimal model, we implement it in an intuitive interface that enables users to enter reactants and obtain predictions for the final products.