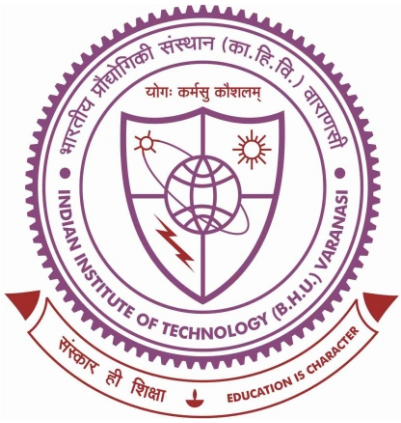
A STUDY OF TOPOLOGICAL INDICES AND THEIR BOUNDS WITH APPLICATIONS TO MOLECULAR GRAPHS



Thesis submitted in partial fulfillment for the Award of the Degree

Doctor of Philosophy

By

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In Figure 7.16, we present the experimental vs expected plot for these 4 physicochemical properties against the AL_1-index.

From the figure, it is pretty evident that the error (less than 0.37) between the experimental and expected values is significantly less for the $logSw$, $logP$ and $logYw$ and the TSA has higher correlation of 99% which is significant high even though the error of 2.25 for a F value of 13360 is insignificant.

7.5 Summary

This chapter has introduced eight new topological indices labeled as AL_1 to AL_8. We also have provided an easy method for computation of AL and VDB indices with the help of neighborhood matrix NM. We have studied the discriminative power of the proposed AL indices and compared the results with a few of the existing VDB indices. Among all the considered indices, four indices, namely AL_4, AL_5, AL_7, and AL_8 have shown the highest discriminative power on the set of octane isomers. The indices AL_4 and AL_7 have the highest discriminative power on the set of PCB molecules compared to the other VDB indices. Further, the degeneracy study finds that the AL indices perform much better than the existing VDB indices in general.

Secondly, we also studied the correlation of AL indices with octane isomers and PCBs' physicochemical properties by fitting a linear regression curve for the data. As a result, we obtained that among all the proposed indices, AL_1 index correlates well with many physicochemical properties and that it exceeds the well-studied Randić index in all such cases. In particular, from the data, we find that AL_1 index has better-predicting power for acentric factor and entropy of octane isomers with a correlation value of 0.97 and 0.95, respectively. Similarly, for the PCBs, we find that AL_1 index has better predictive power for total surface area, log-water-solubility, relative retention time, octanol-water-partition, and log-water-activity coefficients with a correlation value of 0.997, 0.96, 0.95, 0.92, and 0.90, respectively.

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