The Effect of Point Group Symmetry on QSPR of Boiling Point

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This study was conducted to determine the effect of point group symmetry on the QSPR of the boiling points of haloalkanes. Once the point group symmetries of 90 haloalkanes were identified, all the molecules were imported as CML files into Bioclipse-R, an open source QSPR/QSAR software. Bioclipse-R was then used to generate values for 44 descriptors; as many had multiple outputs, this resulted in over 170 descriptor values for each molecule. All of this information was imported into Mathematica for statistical analysis. Linear regression analysis was used to compare the descriptors to the boiling points of the haloalkanes and the descriptors with the five highest R-squared values were reported and compared for all the molecules together, the C_1 point group, the C_S point group, and the C_{3v} point group. The polarizability of a given haloalkane was the most correlated property to the boiling point regardless of point group; however, the ranking of the descriptors which in some way reported the polarizabilities of the molecules did change between the point groups. Thus, point group symmetry does have a slight effect on the QSPR of boiling point for haloalkanes. Predictive QSPR models that incorporate differences between point groups for molecules should be more accurate than those that do not, but the increase in accuracy is likely marginal at best.