Abstract

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Varmuza K., Dehmer M., Emmert-Streib F., Filzmoser P.:

Automorphism groups of alkane graphs.

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The complete set of 618047 isomers of the alkanes with 4 to 20 carbon atoms has been created. From all isomers the automorphism groups have been calculated and evaluated in terms of size, number of asymmetric carbon atoms, and numeric properties of atom and bond orbits.

The presence of a symmetric bond is related to the number of atom and bond orbits.

Molecular descriptors based on automorphism data have been studied, including the known symmetry index, an entropy measure and the root of an orbit polynomial. These descriptors are closely related to the presence of symmetric substructures. The prediction performance of QSPR models for three molecular properties of alkanes and using binary substructure descriptors, is improved by adding descriptors based on automorphism data.