Software SubMat **Application: Automorphism of chemical structure graphs** 210910a

Introduction

Constitutionally (or topologically) **equivalent atoms (bonds)** have the same neighborhood in terms of connectivity given by atom (bond) types and form an **orbit**.

The complete information for this is contained in the **automorphism group** of a graph representing the molecular structure. Automorphism means: **mapping** a graph onto itself while not cutting any bonds.

The size of the automorphism group (α) is the number of possible mappings; it is a symmetry measure for the graph. Asymmetric structures have $\alpha = 1$ (only the identity mapping); for highly symmetric structures α may be large.

SubMat computes for each chemical structure in an SDF-input-file the complete automorphism group and related parameters. Results are provided in a text file, containing e. g., size of the automorphism group, atom and bond orbit data, and recognition of asymmetric C-atoms [1].

Chemical structures are processed by SubMat as colored graphs considering the different elements and different bond types (single, double, triple, aromatic).

[1] Varmuza K. et al.: submitted (2021)

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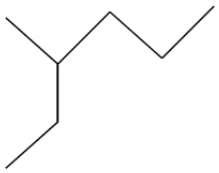
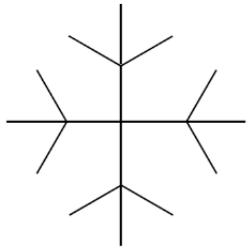
Example: Alkanes

For all 618047 alkane isomers C_4 to C_{20} (trees) the automorphism data have been generated by SubMat [1].



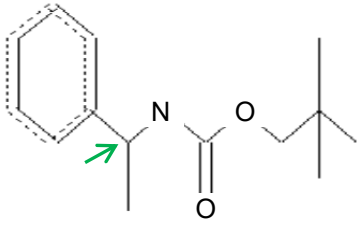
The smallest asymmetric tree has 7 vertices (C_7H_{16}).



An isomer of $C_{17}H_{36}$ has the highest α = 31104.

Example: CNO-compounds

For a set of 2265 structures $C_{0\text{-}18}N_{0\text{-}6}O_{0\text{-}7}H_z$ (H-depleted, no duplicates) from a mass spectra library the automorphism and orbit data have been computed by SubMat. Computing time 2 s (3.4 GHz processor, MS Windows 10); result file 0.8 MB. α = 1 - 1296; number of asymmetric C-atoms = 0 - 8.



Example: $C_{14}H_{21}NO_2$
Results from SubMat:
α = 12; one asymm. C-atom ↗;
no. atom orbits = 13 (10 with C);
no. bond orbits = 12;
elements, bond types considered.