Detour index of hexagonal chains

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(joint work with Dragan Stevanović)

Hexagonal chains are the graph representations of an important subclass of benzenoid molecules, so-called unbranched catacondensed hydrocarbons. Detour index of a connected graph G is defined as $D^*(G) = \sum_{u,v \in V(G)} d^*(u,v)$, where $d^*(u,v)$ represents the longest simple path between vertices u and v. In this paper we do parametrization of hexagonal chains with characteristic sequence and establish formula for detour index using that sequence. We also prove various lower and upper bounds for detour index of hexagonal chains. In particular, among all hexagonal chains of length n, "straight" chain has minimal and "zigzag" chain has maximal detour index.

References

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