Povzetek

V kemiji je zelo razširjeno vprašanje, v kakšni relaciji sta molekulska struktura in fizikalno-kemijske lastnosti spojine. Odgovor na to vprašanje ni preprost, lahko pa si pomagamo z molekulskimi strukturnimi deskriptorji, ki se jih izračuna iz kemijskega grafa določene spojine in za katere verjamemo, da kažejo pomembne strukturne predstavitve osnovne molekule. S pomočjo strukturnih deskriptorjev se torej opiše ne-numeričen podatek (molekulska struktura) s številom, kar je zelo priročno za nadaljnja raziskovanja. Danes igrajo molekulski deskriptorji pomembno vlogo v znanstvenih raziskavah. Uporabljajo se v modelih na različnih področjih znanosti od toksikologije, analitične kemije, fizikalne kemije, medicinske in farmacevtske kemije, okoljevarstvene študije,... Predvsem je zanimivo napovedovanje lastnosti substanc s pomočjo strukturnih deskriptorjev. V diplomskem delu je obravnavano nekaj najpomembnejših molekulskih deskriptorjev, podane so osnovne definicije in nekateri pomembnejši rezultati, predvsem za ekstremalne vrednosti deskriptorjev. Večja pozornost je namenjena Randićevemu indeksu, ki je eden najbolj znanih in najbolj uporabljanih deskriptorjev. Pregledali smo tudi posplošitve tega deskriptorja, ter njegovo povezavo z invariantami grafa. Kadar govorimo o molekulskih deskriptorjih, je za matematike posebej zanimivo vprašanje, kateri razredi grafov imajo maksimalne in minimalne vrednosti molekulskih deskriptorjev, zato je bolj podrobno preučen problem iskanja minimalne vrednosti Randićevega indeksa in podana je celotna rešitev tega problema.

Math. Subj. Class. (MSC 2000): 05C10, 05C35, 05C90

Ključne besede:
molekulski strukturni deskriptor, topološki indeksi, Randićev indeks, Wienerjev indeks, Szeged indeks, Hosoyev indeks, PI-indeks, Estradov indeks, Zagreb indeksa, Cluj indeks

Keywords:
molecular structural descriptor, topological indices, Randić index, Wiener index, Szeged index, Hosoya index, PI index, Estrada index, Zagreb indices, Cluj index

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