

Molecular descriptors of heteratomic and multiple bonds molecules

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joint work with

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Zagreb, September 2022

country	population [mil.]
Japan	125.8
Mexico	128.9

country	population [mil.]	area [10^3 km^2]
Japan	125.8	378
Mexico	128.9	1964

Motivation

Topological indices of weighted graphs
Corrosion inhibition effectiveness
Wiener index of alkenes and alkadienes

Source: <https://en.wikipedia.org/wiki/>



country	population [mil.]	area [10^3 km^2]	density [people per km^2]
Japan	125.8	378	333
Mexico	128.9	1964	66

Motivation

Topological indices of weighted graphs
Corrosion inhibition effectiveness
Wiener index of alkenes and alkadienes

The Elder Wand



The Elder topological index

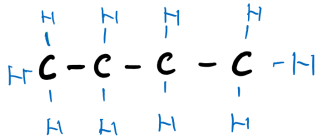
H. Wiener (1947)

The *Wiener index* is the sum of distances between all pairs of vertices

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v)$$

Prediction of boiling points of alkane series

$$T_B(G) = a \cdot W(G) + b \cdot p + c$$

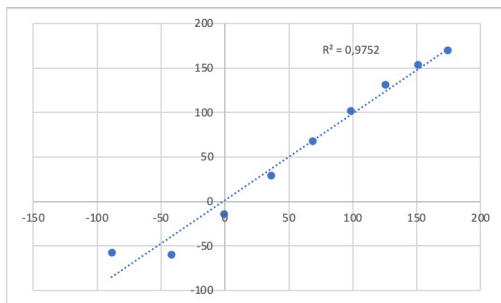


$$W(G) = 1 \cdot 3 + 2 \cdot 2 + 1 \cdot 3 = 10$$

$$p = 1$$

Boiling points of alkane series

alkane	boiling point $T_b [^{\circ}C]$	predicted boiling point $\hat{T}_b [^{\circ}C]$
ethane	-88,6	-57,3
propane	-42,1	-59,6
butane	-0,5	-13,9
pentane	36,1	28,8
hexane	68,9	67,7
heptane	98,4	102,0
octane	125,7	131,0
nonane	150,8	154,0
decane	174,1	170,1

Experimentally determined T_b VS predicted \hat{T}_b 

Weighted graphs

$w : V(G) \rightarrow \mathbb{R}_0^+ \rightarrow (G, w)$ *vertex-weighted graph*

$w' : E(G) \rightarrow \mathbb{R}_0^+ \rightarrow (G, w')$ *edge-weighted graph*

Distance based TI in vertex-weighted graphs

distance $d(u, v)$ is the length of a shortest path between u and v

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Wiener index [Klavžar, Gutman-1997]

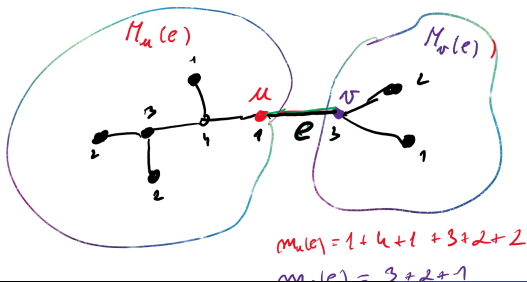
$$W(G, w) = \sum_{\{u,v\} \subseteq V(G)} w(u)w(v)d(u, v).$$

Distance based TI of vertex-weighted graphs

$$M_u(e) = \{x \in V(G) \mid d(u, x) < d(v, x)\}$$

$$M_v(e) = \{x \in V(G) \mid d(v, x) < d(u, x)\}$$

$$m_u(e) = \sum_{x \in M_u(e)} w(x), \quad m_v(e) = \sum_{x \in M_v(e)} w(x)$$



Distance based TI of vertex-weighted graphs

Szeged index [Gutman- 1994]

$$Sz(G, w) = \sum_{e=uv \in E(G)} m_u(e)m_v(e)$$

Degree based TI in vertex-weighted graphs

- *open neighbourhood* N_u is the set of vertices that are adjacent to u
- *degree* of a vertex u in (G, w) is the sum of **weights** of vertices in $N(u)$:

$$\deg(u) = \sum_{v \in N(u)} w(v)$$

Degree based TI in vertex-weighted graphs

first Zagreb index [Gutman, Trinajstić -1997]

$$M_1(G, w) = \sum_{u \in V(G)} (\deg(u))^2$$

second Zagreb index [Gutman, Trinajstić-1997]

$$M_2(G, w) = \sum_{e=uv \in E(G)} \deg(u) \deg(v)$$

Degree based TI in vertex-weighted graphs

Randić index [Randić -1975]

$$R(G, w) = \sum_{e=uv \in E(G)} \frac{1}{\sqrt{\deg(u) \deg(v)}}$$

ABC index [Estrada et al. -1998]

$$ABC(G, w) = \sum_{e=uv \in E(G)} \sqrt{\frac{\deg(u) + \deg(v) - 2}{\deg(u) \deg(v)}}$$

Degree and distance based TI in vertex-weighted graphs

Schultz index [Schultz-1989, Dobrynin et al.-1993]

$$DD(G, w) = \sum_{\{u,v\} \subseteq V(G)} (\deg(u) + \deg(v))d(u, v)$$

Gutman index [Gutman-1994]

$$Gut(G, w) = \sum_{\{u,v\} \subseteq V(G)} \deg(u)\deg(v)d(u, v)$$

Adjacency matrix of a vertex-weighted graph

$$A(G, w)_{ij} = \begin{cases} 1 & ; v_i v_j \in E(G, w) \\ 0 & ; v_i v_j \notin E(G, w) \\ w(v_i) & ; v_i = v_j \end{cases}$$

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$\lambda_1, \lambda_2, \dots, \lambda_n$ eigenvalues of $A(G, w)$

Eigenvalues based TI in vertex-weighted graphs

graph energy [Li, Shi, Gutman - 2012]

$$E(G, w) = \sum_{i=1}^n |\lambda_i|$$

Estrada index [Estrada - 2000]

$$EE(G, w) = \sum_{i=1}^n e^{\lambda_i}$$

Gaussian Estrada index [Estrada et al. - 2017]

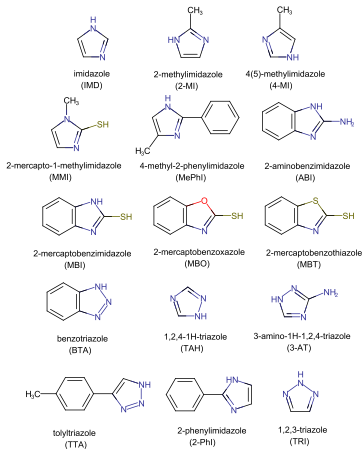
$$GEE(G, w) = \sum_{i=1}^n e^{-\lambda_i^2}$$

Corrosion of metals



Source: www.dynagard.info

Corrosion inhibitors



Corrosion inhibition effectiveness

$$\text{IE} [\%] = 100 \frac{\Delta m_{\text{without inhibitor}} - \Delta m_{\text{with inhibitor}}}{\Delta m_{\text{without inhibitor}}}$$

Experimentally measured IE's for 15 corrosion inhibitors

Corr.inh.	IE ₁	IE ₂	IE ₃	IE ₄	IE ₅	IE ₆	IE ₇	IE ₈
IMD	2.05	11.02	2.05	24.15	-6.15	30.82	-33.94	-24.84
2-MI	-10.71	20.82	7.97	31.41	-1.14	23.37	-19.82	3.77
4-MI	-9.34	18.86	8.43	26.70	-9.34	22.20	-27.56	9.85
MMI	19.36	12.00	7.52	25.72	-18.91	29.45	-14.81	12.98
MePhI	-17.08	20.43	-0.23	24.55	-19.82	26.70	-35.76	-0.15
ABI	3.42	14.55	-3.42	28.07	0.23	28.27	-17.08	9.65
MBI	-0.68	-5.24	-23.92	13.18	-26.20	6.32	-11.16	13.38
MBO	1.59	-20.14	-7.97	18.86	-38.95	-195.74	10.25	26.51
MBT	7.52	-7.99	-23.01	-5.05	-12.98	-0.15	-34.85	-2.50
BTA	26.20	9.06	17.08	27.49	3.87	22.78	11.16	18.86
TAH	11.16	-24.64	-0.23	-16.22	-6.61	-14.45	5.69	0.44
3-AT	12.07	-7.20	-12.07	-1.91	-18.91	-7.01	-10.71	14.75
TTA	12.98	15.14	17.54	24.94	19.82	20.24	17.08	17.10
2-PhI	-10.71	16.12	-6.61	22.59	-13.44	30.03	-12.98	-20.33
TRI	-1.59	-26.21	-36.22	-61.10	-44.42	-69.33	-48.06	-88.93

Periodic table

PERIODIC TABLE OF ELEMENTS

1 H Hydrogen Nonmetal																	2 He Helium Noble Gas						
3 Li Lithium Alkali Metal	4 Be Beryllium Alkaline Earth Metal																	5 B Boron Metalloid	6 C Carbon Nonmetal	7 N Nitrogen Nonmetal	8 O Oxygen Nonmetal	9 F Fluorine Halogen	10 Ne Neon Noble Gas
11 Na Sodium Alkali Metal	12 Mg Magnesium Alkaline Earth Metal																	13 Al Aluminum Poor Metal	14 Si Silicon Metalloid	15 P Phosphorus Nonmetal	16 S Sulfur Nonmetal	17 Cl Chlorine Halogen	18 Ar Argon Noble Gas
19 K Potassium Alkali Metal	20 Ca Calcium Alkaline Earth Metal	21 Sc Scandium Transition Metal	22 Ti Titanium Transition Metal	23 V Vanadium Transition Metal	24 Cr Chromium Transition Metal	25 Mn Manganese Transition Metal	26 Fe Iron Transition Metal	27 Co Cobalt Transition Metal	28 Ni Nickel Transition Metal	29 Cu Copper Transition Metal	30 Zn Zinc Transition Metal	31 Ga Gallium Poor Metal	32 Ge Germanium Metalloid	33 As Arsenic Metalloid	34 Se Selenium Nonmetal	35 Br Bromine Halogen	36 Kr Krypton Noble Gas						
37 Rb Rubidium Alkali Metal	38 Sr Strontium Alkaline Earth Metal	39 Y Yttrium Transition Metal	40 Zr Zirconium Transition Metal	41 Nb Niobium Transition Metal	42 Mo Molybdenum Transition Metal	43 Tc Technetium Transition Metal	44 Ru Ruthenium Transition Metal	45 Rh Rhodium Transition Metal	46 Pd Palladium Transition Metal	47 Ag Silver Transition Metal	48 Cd Cadmium Transition Metal	49 In Indium Poor Metal	50 Sn Tin Poor Metal	51 Sb Antimony Metalloid	52 Te Tellurium Metalloid	53 I Iodine Halogen	54 Xe Xenon Noble Gas						
55 Cs Cesium Alkali Metal	56 Ba Barium Alkaline Earth Metal	•	72 Hf Hafnium Transition Metal	73 Ta Tantalum Transition Metal	74 W Tungsten Transition Metal	75 Re Rhenium Transition Metal	76 Os Osmium Transition Metal	77 Ir Iridium Transition Metal	78 Pt Platinum Transition Metal	79 Au Gold Transition Metal	80 Hg Mercury Transition Metal	81 Tl Thallium Poor Metal	82 Pb Lead Poor Metal	83 Bi Bismuth Metalloid	84 Po Polonium Metalloid	85 At Astatine Halogen	86 Rn Radon Noble Gas						
87 Fr Francium Alkali Metal	88 Ra Radium Alkaline Earth Metal	••	104 Rf Rutherfordium Transition Metal	105 Db Dubnium Transition Metal	106 Sg Seaborgium Transition Metal	107 Bh Bohrium Transition Metal	108 Hs Hassium Transition Metal	109 Mt Meitnerium Transition Metal	110 Ds Darmstadtium Transition Metal	111 Rg Roentgenium Transition Metal	112 Cn Copernicium Transition Metal	113 Nh Nihonium Poor Metal	114 Fl Flerovium Poor Metal	115 Mc Moscovium Metalloid	116 Lv Livermorium Metalloid	117 Ts Tennessine Halogen	118 Og Oganesson Noble Gas						
•	•	•	57 La Lanthanum Lanthanide	58 Ce Cerium Lanthanide	59 Pr Praseodymium Lanthanide	60 Nd Neodymium Lanthanide	61 Pm Promethium Lanthanide	62 Sm Samarium Lanthanide	63 Eu Europium Lanthanide	64 Gd Gadolinium Lanthanide	65 Tb Terbium Lanthanide	66 Dy Dysprosium Lanthanide	67 Ho Holmium Lanthanide	68 Er Erbium Lanthanide	69 Tm Thulium Lanthanide	70 Yb Ytterbium Lanthanide	71 Lu Lutetium Lanthanide						
•	•	•	89 Ac Actinium Actinide	90 Th Thorium Actinide	91 Pa Protactinium Actinide	92 U Uranium Actinide	93 Np Neptunium Actinide	94 Pu Plutonium Actinide	95 Am Americium Actinide	96 Cm Curium Actinide	97 Bk Berkelium Actinide	98 Cf Californium Actinide	99 Es Einsteinium Actinide	100 Fm Fermium Actinide	101 Md Mendelevium Actinide	102 No Nobelium Actinide	103 Lr Lawrencium Actinide						

1
H
Hydrogen
Nonmetal

Atomic Number
Symbol
 Name
 Chemical Group Block



4 models of vertex-weighted molecular graphs

Atom	Model 1	Model 2	Model 3	Model 4
C arbon	1	1	6	1
N itrogen	1	7	7	7/6
O xygen	1	8	8	4/3
S ulfur	1	16	16	8/3

Data

- 15 corrosion inhibitors
- 8 types of corrosion inhibition effectiveness obtained experimentally
- 4 models for determination of weights of vertices in (G, w)
- 8 topological indices

Tools for calculations

- Input: (weighted) adjacency matrices for 15 molecules

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- topological indices are calculated by programming in Sage
- regression analysis is done in programme R

Best results

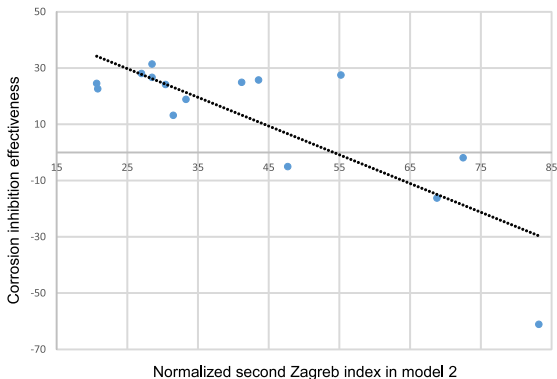


Figure: The linear regression between M_2^2/n and IE_4 , $R = -0.81$.

Best results

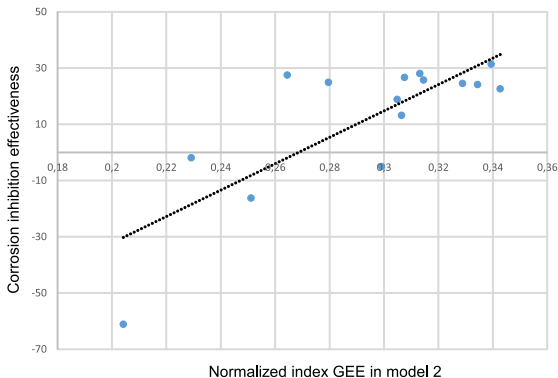


Figure: The linear regression between GEE^2/n and IE_4 , $R = 0.78$.

Multiple bonds molecules

edge-weighted graphs (G, w')



alkene



alkadiene

Wiener index of (G, w')

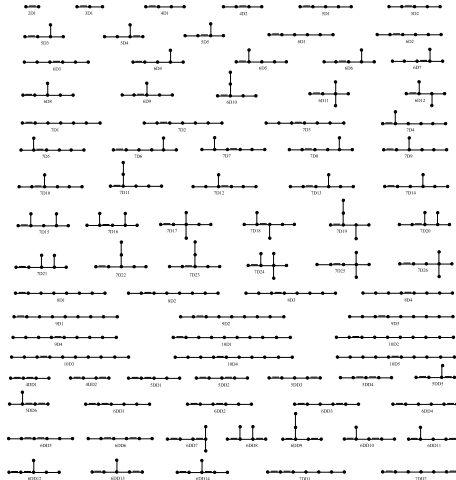
Wiener index of (G, w') [Klavžar, Nadjafi-Aranni - 2013]

$$W(G, w') = \sum_{\{u,v\} \subseteq V(G)} d_{(G,w')}(u, v)$$

shortest path P between u and v of (G, w') is a path with the minimum weight $w'(P)$ among all possible paths between u and v :

$$d_{(G,w')}(u, v) = w'(P)$$

Molecules-alkenes and alkadienes



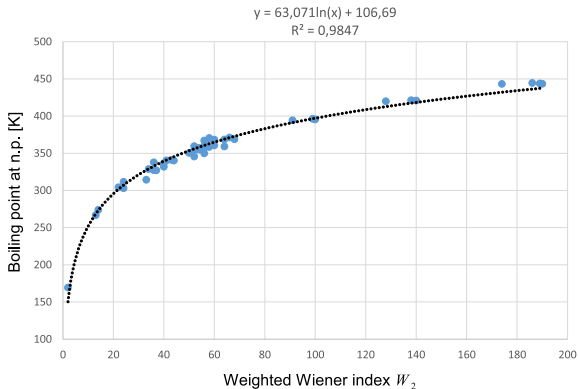
What is the weight of double-bond?

1, 2, $\frac{1}{2}$ or actual bond length

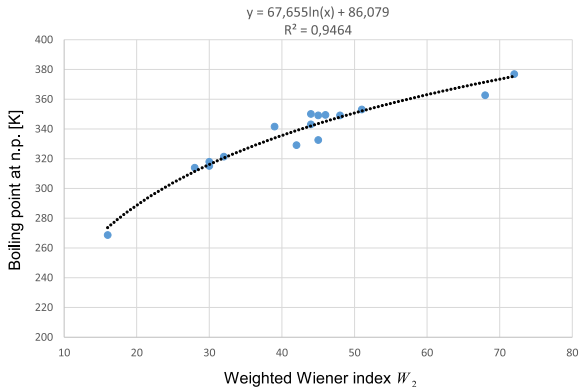
Bonds lengths

Bond Type	Bond Length	Relative Distance
$sp^3 - sp^3$	1.544	1.000
$sp^3 - sp^2$	1.501	0.972
$sp^2 - sp^2$	1.483	0.960
$sp^2 - sp^2 + \pi$	1.339	0.867
$sp^2 - sp + \pi$	1.309	0.848

Wiener index of alkenes with $w(e) = 2$



Wiener index of alkadienes with $w(e) = 2$



THE END...thanks