Molecular descriptors of heteratomic and multiple bonds molecules

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joint work with

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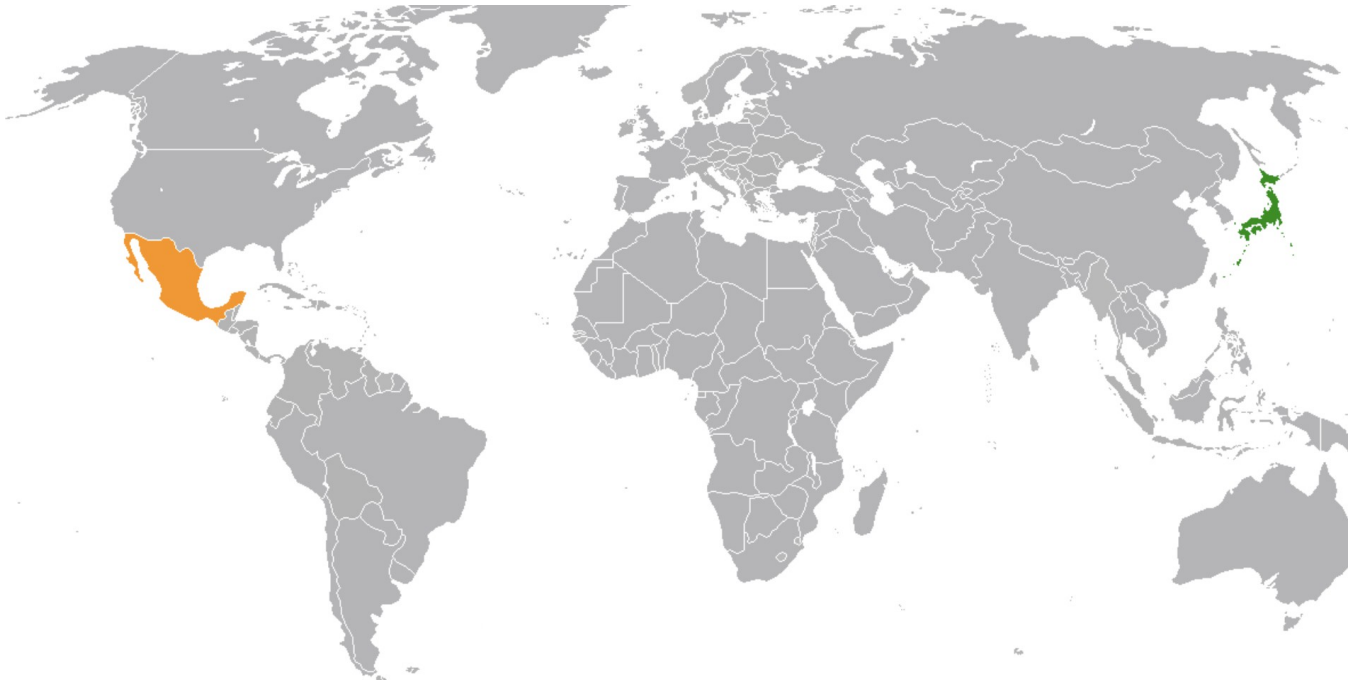
country	population [mil.]
Japan	125.8
Mexico	128.9

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

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**

The Elder Wand

The Elder topological index

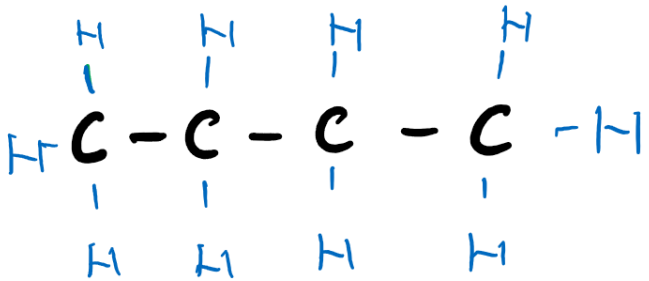
H. Wiener (1947)

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

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

Prediction of boiling points of alkane series

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



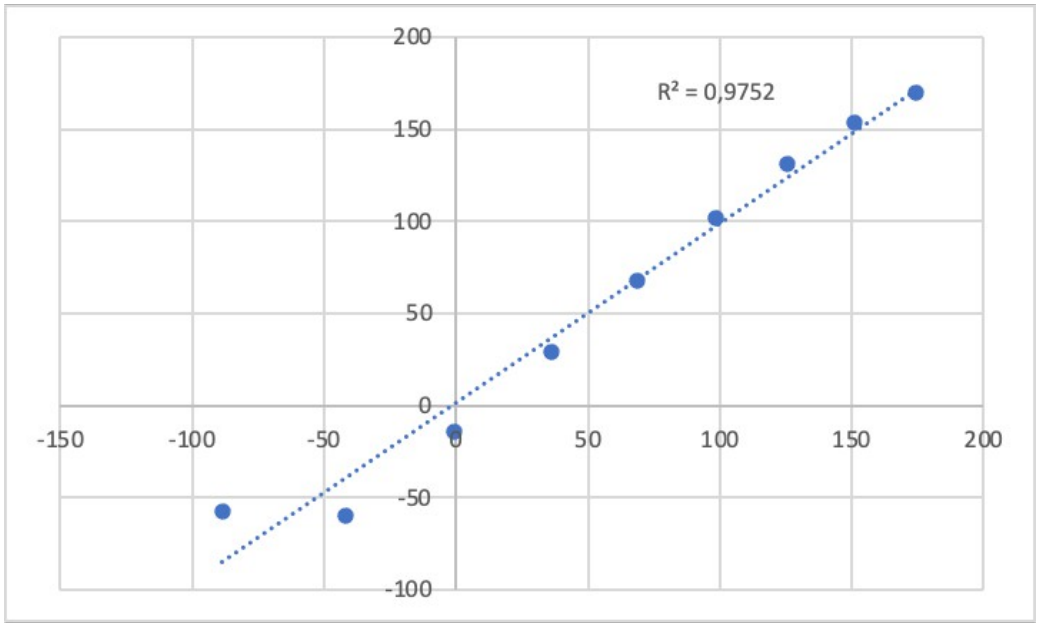
$W(G) = 1 \cdot 3 + 2 \cdot 2 + 1 \cdot 3 = 10$

$p = 1$

Boiling points of alkane series

alkane	boiling point $T_b\,[^\circ C]$	predicted boling point $\widehat{T}_b\,[^\circ C]$
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

Experimentaly determined T_b vs predicted $\widehat{T}_b$



Weighted graphs

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

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

Distance based TI in vertex-weighted graphs

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

Distance based TI in vertex-weighted graphs

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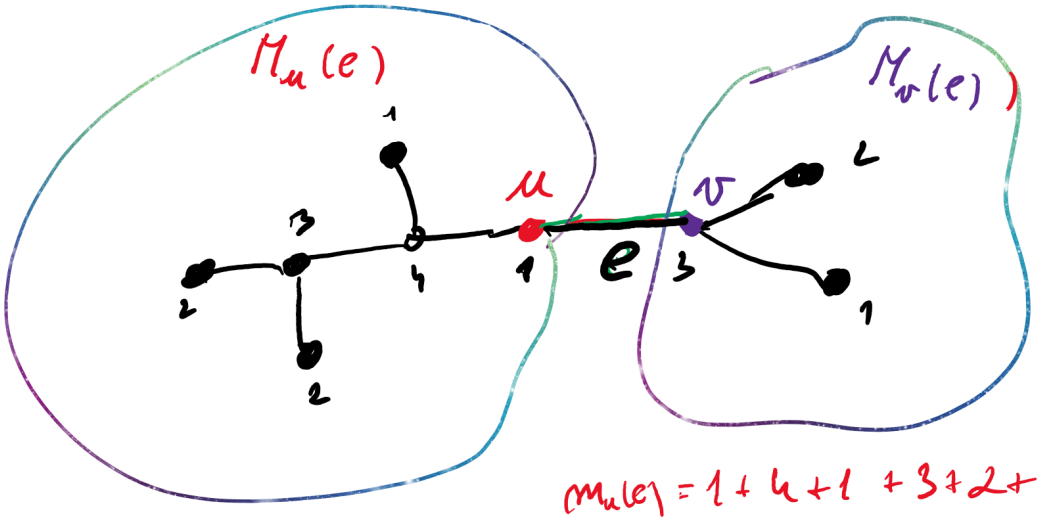
Wiener index [Klavžar, Gutman-1997]

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

Distance based TI of vertex-weighted graphs

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

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



$m_u(e) = 1 + 4 + 1 + 3 + 2 + 2$

$m_v(e) = 3 + 2 + 1$

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

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

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

Eigenvalues based TI in vertex-weighted graphs

graph energy [Li, Shi, Gutman - 2012]

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

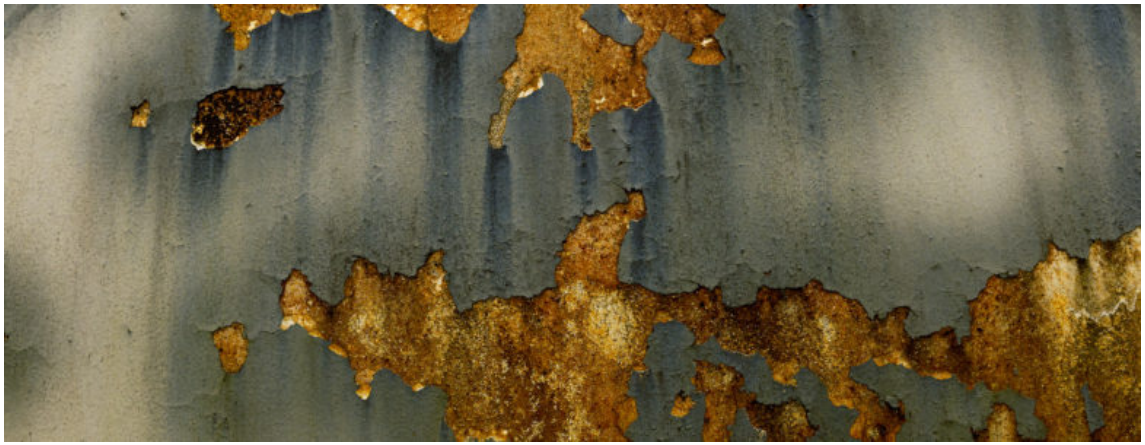
Estrada index [Estrada - 2000]

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

Gaussian Estrada index [Estrada et al. - 2017]

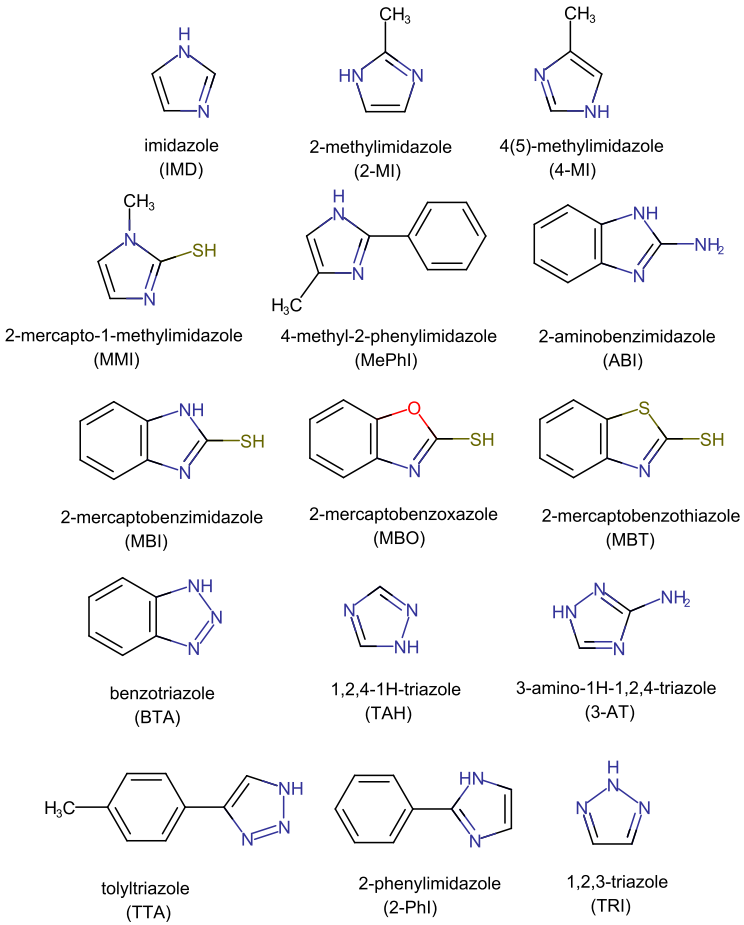
$$GEE(G,w) = \sum_{i=1}^{n} e^{-\lambda_i^2}$$

Corrosion of metals



Source: www.dynagard.info

Corrosion inhibitors



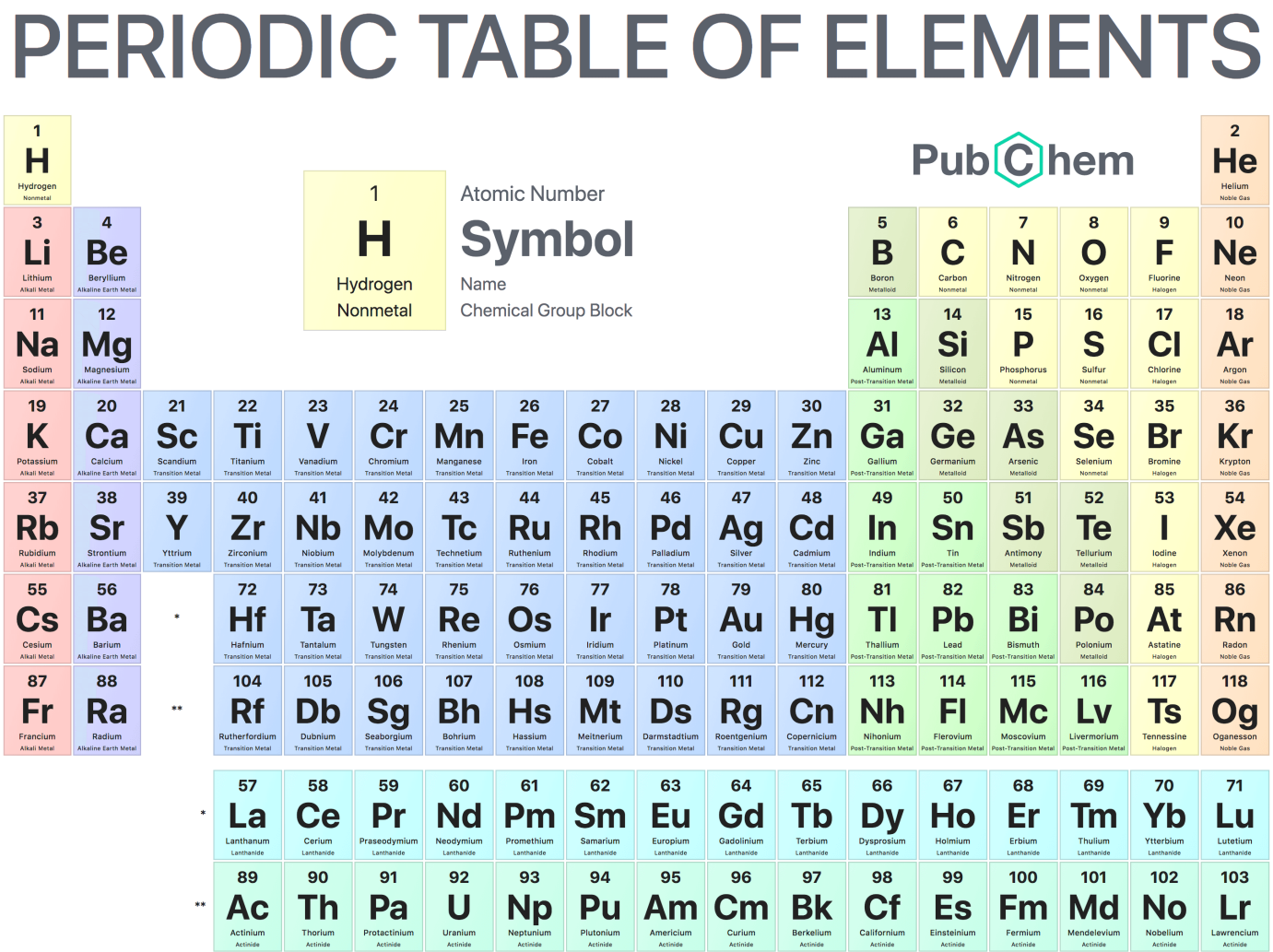
Corrosion inhibition effectiveness

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

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



4 models of vertex-weighted molecular graphs

Atom	Model 1	Model 2	Model 3	Model 4
Carbon	1	1	6	1
Nitrogen	1	7	7	7/6
Oxygen	1	8	8	4/3
Sulfur	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

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- regression analysis is done in programme R

Best results

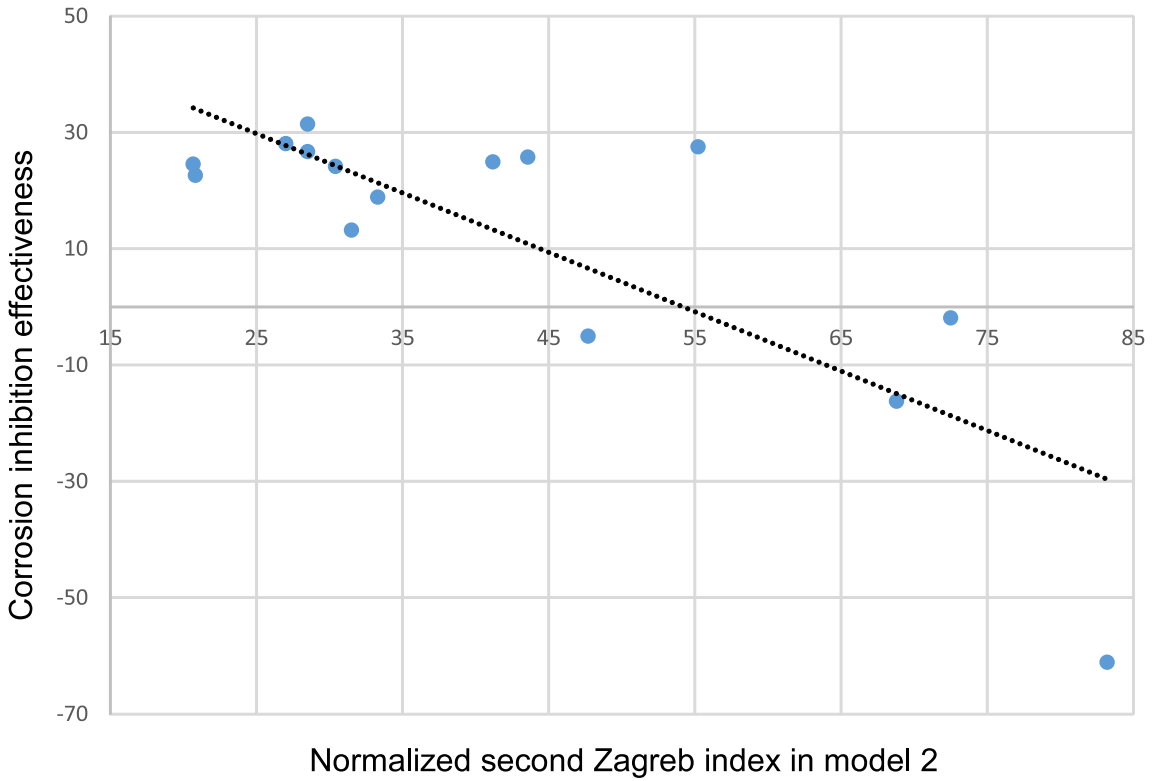


Figure: The linear regression between M_2^2/n and IE_4, $R = -0.81$.

Best results

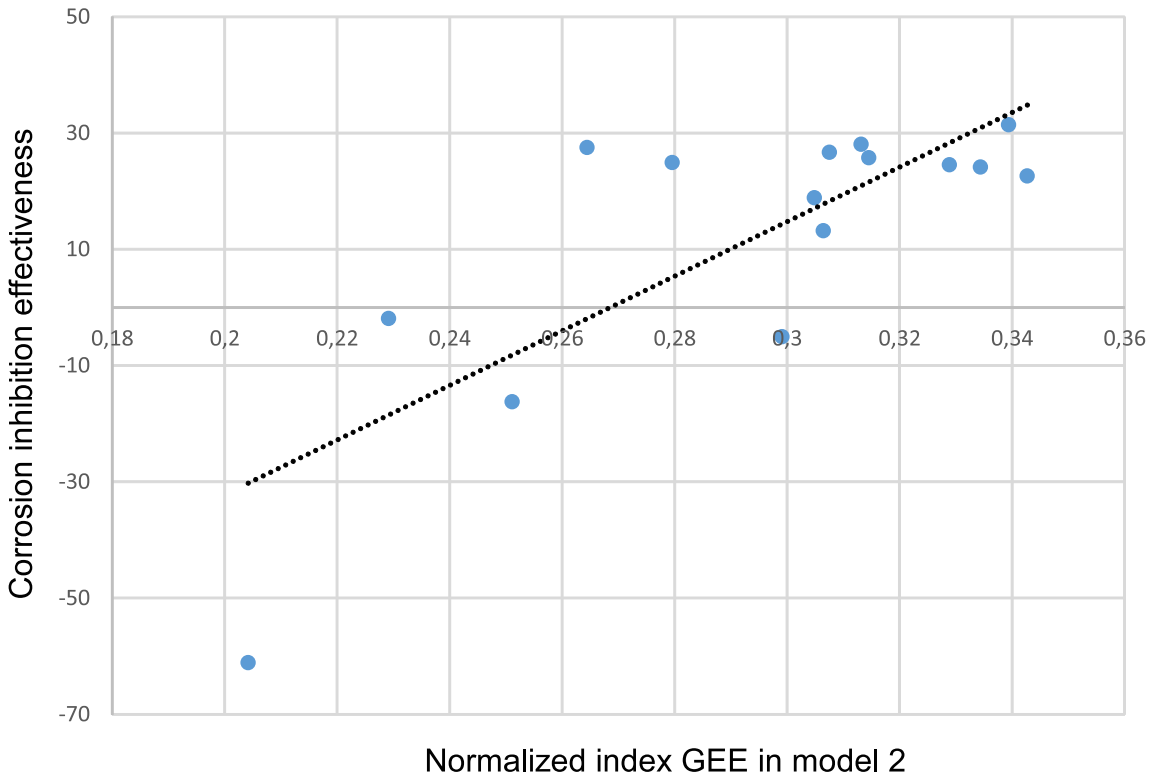


Figure: The linear regression between GEE^2/n and IE_4, $R = 0.78$.

Multiple bonds molecules

edge-weighted graphs (G, w')

alkene

alkadiene

Wiener index of (G, w')

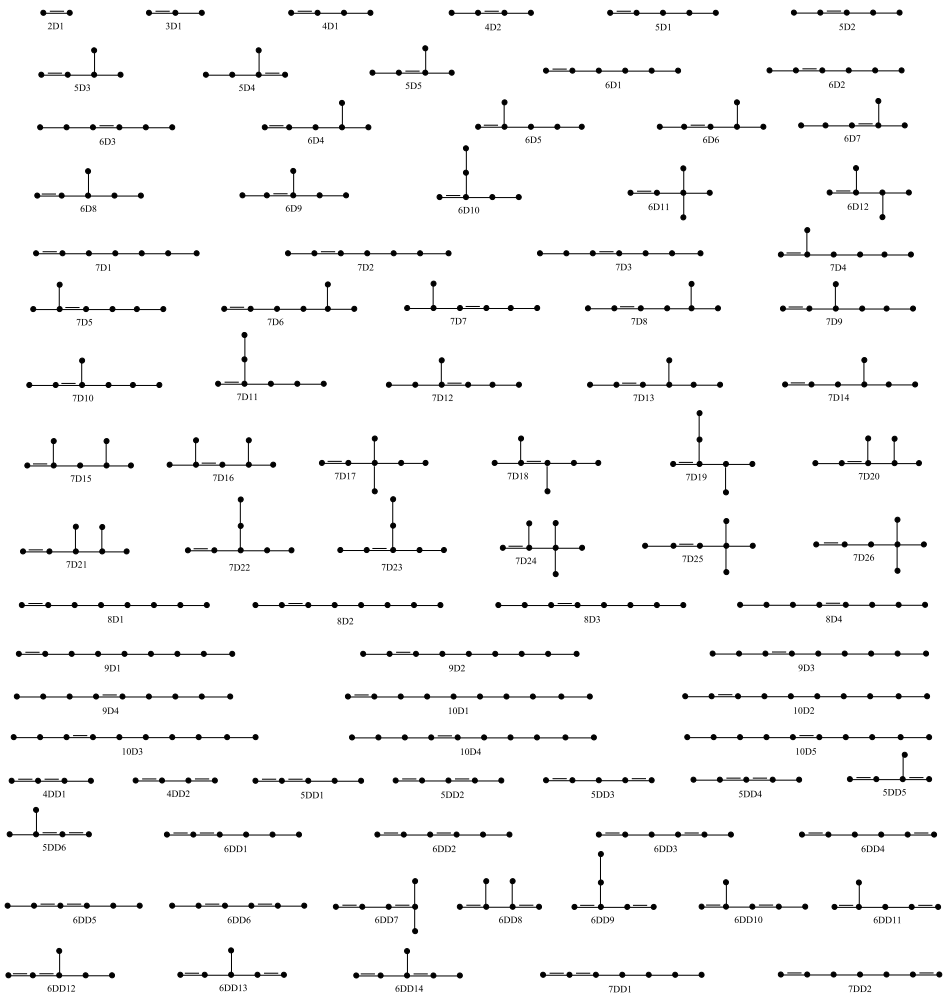
Wiener index of (G, w') [Klavžar, Nadjafi-Aranni - 2013]

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

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?

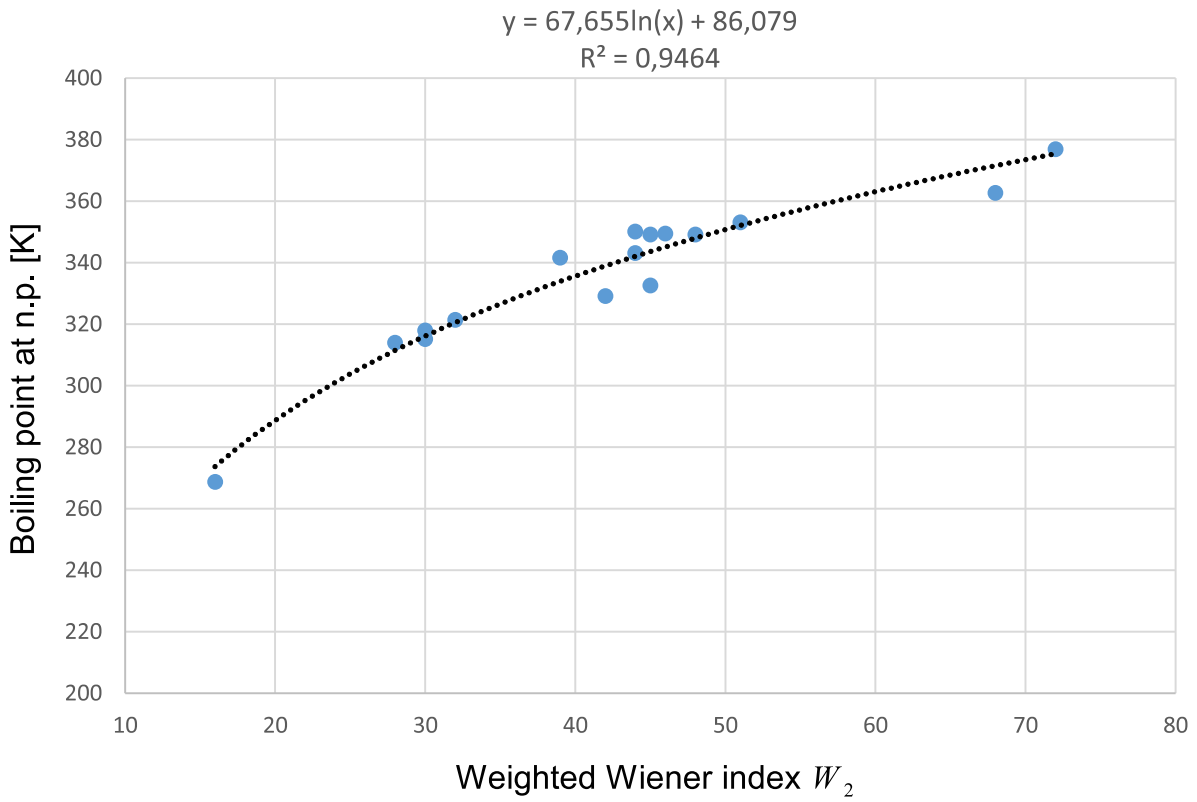
$$1, \quad 2, \quad \frac{1}{2} \quad \text{or actual bond length}$$

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