

Topological Index Calculator Manual

Created by Steven Granz - June 2004
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Overview:

Since the development of the Wiener Index, numerous topological indices have been described. These methods convert molecular structure to a mathematical representation (a chemical graph) and then define computations to be performed on the resulting graph. Statistical correlations between those results and physical properties serve as a predictive tool. In organic chemistry, students are taught the relationship between molecular structure and boiling point but generally do not investigate the phenomenon because tools to support the tedious calculations are lacking.

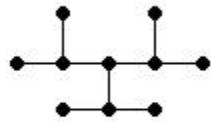
Topological Index Calculator is a freely available JavaScript application for the computation of QSPR descriptor indices for alkane molecules. The current program supports the computation of the following indices: Polarity Index, Weiner Index, Balaban Index, Odd-Even Index, Vertex Degree Distance Index, Harary Index, Randic and Hosoya Index. Use of JavaScript benefits instructors who may wish to modify or extend the program's capabilities and students who may want to use the tool easily both in and out of the laboratory. With this program, students may work cooperatively to develop correlations between topological indices and physical properties of alkanes.

Compute Topological Indices using an Edge List:

1. Chemical graphs are mathematical objects that represent chemical compounds. In chemical graphs, vertices correspond to atoms and edges represent covalent bonds between atoms. Topological indices are a convenient way for expressing in a numerical form the chemical structure of chemical structure encoded in the chemical graphs.
2. Create a chemical graph to represent the molecule.

Example:

2,4-dimethyl-3-isopropylpentane



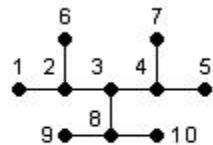
3. Label all vertices from 1 to n; where n = number of carbon atoms.

Example:

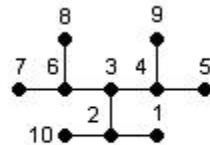
2,4-dimethyl-3-isopropylpentane

$$n = 10$$

Graph 1



Graph 2



Note: It does not matter what order we label the vertices. Both of these graphs will produce the same value for the indices.

4. Create a list of all connections between two vertices.

Example:

Graph 1

1	2
2	3
3	4
4	5
2	6
4	7
3	8
8	9
8	10

Graph 2

1	2
2	3
3	4
4	5
4	9
2	10
3	6
6	7
6	8

5. Open Topological Index Calculator into your favorite JavaScript enabled web browser.

www.math-CS.gordon.edu/courses/organic/topo

Topological Index Calculator

Select parent chain or ring

C1, methane

Bonds:

- | | |
|--------------------------------------------------|------------------------|
| <input type="checkbox"/> Polarity: | <input type="text"/> ? |
| <input type="checkbox"/> Weiner: | <input type="text"/> ? |
| <input type="checkbox"/> Hosoya: | <input type="text"/> ? |
| <input type="checkbox"/> Randic: | <input type="text"/> ? |
| <input type="checkbox"/> Balaban: | <input type="text"/> ? |
| <input type="checkbox"/> Harary: | <input type="text"/> ? |
| <input type="checkbox"/> Vertex Degree Distance: | <input type="text"/> ? |
| <input type="checkbox"/> Odd-Even: | <input type="text"/> ? |

SMILES: [?](#)

[**What is a Topological Index?**](#)

[**Manual**](#)

Data:

6. It is convenient to determine the parent chain or ring of the molecule in order to automatically enter some of the connections. If we have the name of the molecule, the last part of the name is the parent chain or ring.

Example:

3,3-dimethylbicyclo[3.3.0]octane – octane is our parent ring.
2,4-dimethyl-3-isopropylpentane – pentane is our parent chain.

If we do not have the name of the molecule then we will need to manually enter all the connections.

7. Select either the parent chain or ring and click on the drop down menu and select the appropriate parent.

Topological Index Calculator

Select parent chain or ring:

C5, pentane
C1, methane
C2, ethene
C3, propane
C4, butane
C5, pentane
C6, hexane
C7, heptane
C8, octane
C9, nonane
C10, decane
C11, undecane
C12, dodecane
C13, tridecane
C14, tetradecene
C15, pentadecane
C16, hexadecane
C17, heptadecane
C18, octadecane
C19, nonadecane
C20, icosane

Polarity: ?
 Weiner: ?
 Hosoya: ?
 Randic: ?
 Balaban: ?
 Harary: ?
 Vertex Degree Distance: ?
 Odd-Even: ?

SMILES: ?

[What is a Topological Index?](#) [Manual](#)

Data:

Topological Index Calculator

Select parent chain or ring

C5, pentane

Bonds:

1 2
2 3
3 4
4 5

- | | | |
|--------------------------------------------------|----------------------|---|
| <input type="checkbox"/> Polarity: | <input type="text"/> | ? |
| <input type="checkbox"/> Weiner: | <input type="text"/> | ? |
| <input type="checkbox"/> Hosoya: | <input type="text"/> | ? |
| <input type="checkbox"/> Randic: | <input type="text"/> | ? |
| <input type="checkbox"/> Balaban: | <input type="text"/> | ? |
| <input type="checkbox"/> Harary: | <input type="text"/> | ? |
| <input type="checkbox"/> Vertex Degree Distance: | <input type="text"/> | ? |
| <input type="checkbox"/> Odd-Even: | <input type="text"/> | ? |

Compute

Clear Bonds

Add Data Line

SMILES: ?

Convert Edge List to SMILES

Compute using SMILES

Convert SMILES to Edge List

[What is a Topological Index?](#)

[Manual](#)

Data:

Clear Console

8. Now we need to add the remaining connections into the bonds field.
The format required for a pair is a number, a space, a number and a return.

Example:

[Graph 1](#)

Topological Index Calculator

Select parent chain or ring:

C5, pentane

Bonds:

1 2
2 3
3 4
4 5
2 6
4 7
3 8
8 9
8 10

- Polarity: ?
- Weiner: ?
- Hosoya: ?
- Randic: ?
- Balaban: ?
- Harary: ?
- Vertex Degree Distance: ?
- Odd-Even: ?

SMILES: [?](#)

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Data:

[Graph 2](#)

Topological Index Calculator

Select parent chain or ring

C1, methane

Bonds:

1 2
2 3
3 4
4 5
4 9
2 10
3 6
6 7
6 8

- Polarity: ?
- Weiner: ?
- Hosoya: ?
- Randic: ?
- Balaban: ?
- Harary: ?
- Vertex Degree Distance: ?
- Odd-Even: ?

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Data:

9. Check the indices that we wish to compute. Click the Compute button to calculate the indices.

Note: The edge list must be an acyclic alkane to compute the Hosoya Index or an error message will be shown.

Example:

Graph 1

Topological Index Calculator

Select parent chain or ring:
C5, pentane

Bonds:

1 2	<input checked="" type="checkbox"/> Polarity:	12
2 3	<input checked="" type="checkbox"/> Weiner:	117
3 4	<input checked="" type="checkbox"/> Hosoya:	54
4 5	<input checked="" type="checkbox"/> Randic:	4.4641
2 6	<input checked="" type="checkbox"/> Balaban:	3.9835
4 7	<input checked="" type="checkbox"/> Harary:	14.0833
3 8	<input checked="" type="checkbox"/> Vertex Degree Distance:	5.8832
8 9	<input checked="" type="checkbox"/> Odd-Even:	13.1667
8 10		

Compute Clear Bonds Add Data Line

SMILES: [?](#)

Convert Edge List to SMILES

Compute using SMILES Convert SMILES to Edge List

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Data:

Clear Console

Graph 2

Topological Index Calculator

Select parent chain or ring

C5, pentane

Bonds:

1 2
2 3
3 4
4 5
4 9
2 10
3 6
6 7
6 8

<input checked="" type="checkbox"/> Polarity:	12	?
<input checked="" type="checkbox"/> Weiner:	117	?
<input checked="" type="checkbox"/> Hosoya:	54	?
<input checked="" type="checkbox"/> Randic:	4.4641	?
<input checked="" type="checkbox"/> Balaban:	3.9835	?
<input checked="" type="checkbox"/> Harary:	14.0833	?
<input checked="" type="checkbox"/> Vertex Degree Distance:	5.8832	?
<input checked="" type="checkbox"/> Odd-Even:	13.1667	?

[Compute](#)

[Clear Bonds](#)

[Add Data Line](#)

SMILES: [?](#)

[Convert Edge List to SMILES](#)

[Compute using SMILES](#)

[Convert SMILES to Edge List](#)

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Data:

[Clear Console](#)

[Error Example:](#)

Topological Index Calculator

Select parent chain or ring

C5, pentane

Bonds:

1 2
2 3
3 4
4 5
5 1
2 6
4 7
3 8
8 9
8 10

- Polarity: ?
 Weiner: ?
 Hosoya: ?
 Randic: ?
 Balaban: ?
 Harary: ?
 Vertex Degree Distance: ?



Compute

Clear Bonds

Add Data Line

SMILES: [?](#)

Convert Edge List to SMILES

Compute using SMILES

Convert SMILES to Edge List

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Data:

Clear Console

Topological Index Calculator

Select parent chain or ring

C5. pentane

Bonds:

1 2
2 3
3 4
4 5
5 1
2 6
4 7
3 8
8 9
8 10

<input checked="" type="checkbox"/> Polarity:	12	?
<input checked="" type="checkbox"/> Weiner:	110	?
<input checked="" type="checkbox"/> Hosoya:		?
<input checked="" type="checkbox"/> Randic:	4.6259	?
<input checked="" type="checkbox"/> Balaban:	2.5383	?
<input checked="" type="checkbox"/> Harary:	15.3958	?
<input checked="" type="checkbox"/> Vertex Degree Distance:	6.8004	?
<input checked="" type="checkbox"/> Odd-Even:	14.5417	?

[Compute](#)

[Clear Bonds](#)

[Add Data Line](#)

SMILES: [?](#)

[Convert Edge List to SMILES](#)

[Compute using SMILES](#)

[Convert SMILES to Edge List](#)

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[Manual](#)

Data:

[Clear Console](#)

Compute Topological Indices using SMILES:

1. Input the SMILES nomenclature of the molecule into the provided text field.

Topological Index Calculator

Select parent chain or ring

C1, methane

Bonds:

- Polarity: ?
- Weiner: ?
- Hosoya: ?
- Randic: ?
- Balaban: ?
- Harary: ?
- Vertex Degree Distance: ?
- Odd-Even: ?

SMILES: [?](#)

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Data:

Note: The SMILES nomenclature must be a valid acyclic alkane or an error message will be shown.

A valid acyclic alkane:

- Only has the following characters: C ()
- Does not have the following: O ()

- Starts with a C
- Ends with a C
- Has an equal number of open and closing parentheses

Error Example:

Topological Index Calculator

Select parent chain or ring
C1, methane

Bonds:

Polarity: ?
 Weiner: ?
 Hosoya: ?
 Randic: ?
 Balaban: ?
 Harary: ?
 Vertex Degree Distance: ?

[JavaScript Application] x

Please input a valid SMILES nomenclature that represents an acyclic alkane.

OK

Compute Clear Bonds Add Data Line

SMILES: ?
[C1C(C)C(O(C)C)O(C)C1] Convert Edge List to SMILES

Compute using SMILES Convert SMILES to Edge List

[What is a Topological Index?](#) [Manual](#)

Data:

Clear Console

2. Check the indices that we wish to compute. Click the Compute using SMILES button to calculate the indices.

Topological Index Calculator

Select parent chain or ring:

C1, methone

Bonds:

<input checked="" type="checkbox"/> Polarity:	12	?
<input checked="" type="checkbox"/> Weiner:	117	?
<input checked="" type="checkbox"/> Hosoya:	54	?
<input checked="" type="checkbox"/> Randic:	4.4641	?
<input checked="" type="checkbox"/> Balaban:	3.9835	?
<input checked="" type="checkbox"/> Harary:	14.0833	?
<input checked="" type="checkbox"/> Vertex Degree Distance:	5.8832	?
<input checked="" type="checkbox"/> Odd-Even:	13.1667	?

[Compute](#)

[Clear Bonds](#)

[Add Data Line](#)

SMILES: [?](#)

CC(C)O(C(C)C)O(C)C

[Convert Edge List to SMILES](#)

[Compute using SMILES](#)

[Convert SMILES to Edge List](#)

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Data:

[Clear Console](#)

Convert an Edge List to the SMILES Representation:

1. Follow instructions 1-8 in the section: Compute Topological Indices using an Edge List.
2. Click the Convert Edge List to SMILES button to convert an edge list to the SMILES nomenclature.

Note: The edge list must be an acyclic alkane to convert it to SMILES nomenclature or an error message will be shown.

Topological Index Calculator

Select parent chain or ring
C5, pentane

Bonds:

1 2	<input type="checkbox"/> Polarity:	[]
2 3	<input type="checkbox"/> Weiner:	[]
3 4	<input type="checkbox"/> Hosoya:	[]
4 5	<input type="checkbox"/> Randic:	[]
2 6	<input type="checkbox"/> Balaban:	[]
4 7	<input type="checkbox"/> Harary:	[]
3 8	<input type="checkbox"/> Vertex Degree Distance:	[]
8 9	<input type="checkbox"/> Odd-Even:	[]
8 10		

Compute Clear Bonds Add Data Line

SMILES: [?](#)

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Data:

Error Example:

Topological Index Calculator

Select parent chain or ring
C5. pentane

Bonds:

1 2	<input type="checkbox"/> Polarity: ?
2 3	<input type="checkbox"/> Weiner: ?
3 4	<input type="checkbox"/> Hosoya: ?
4 5	<input type="checkbox"/> Randic: ?
5 1	<input type="checkbox"/> Balaban: ?
2 6	<input type="checkbox"/> Harary: ?
4 7	<input type="checkbox"/> Vertex Degree Distance: ?
3 8	
8 9	
8 10	

[JavaScript Application] ×

Please input an edge list that represents an acyclic alkane.

! OK

Compute Clear Bonds Add Data Line

SMILES: [?](#) Convert Edge List to SMILES

Compute using SMILES Convert SMILES to Edge List

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Data:

Clear Console

Convert the SMILES representation to an Edge List

1. Input the SMILES nomenclature of the molecule into the provided text field.

Topological Index Calculator

Select parent chain or ring
C1, methane

Bonds:

- Polarity: ?
- Weiner: ?
- Hosoya: ?
- Randic: ?
- Balaban: ?
- Harary: ?
- Vertex Degree Distance: ?
- Odd-Even: ?

SMILES: [?](#)

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Data:

2. Click the Convert SMILES to Edge List button to convert the SMILES nomenclature to an edge list.

Note: The SMILES nomenclature must be a valid acyclic alkane or an error message will be shown.

Topological Index Calculator

Select parent chain or ring

C1, methane

Bonds:

1 2
2 3
2 4
4 5
5 6
5 7
4 8
6 9
8 10

- Polarity: ?
- Weiner: ?
- Hosoya: ?
- Randic: ?
- Balaban: ?
- Harary: ?
- Vertex Degree Distance: ?
- Odd-Even: ?

SMILES: [?](#)

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[Manual](#)

Data:

[Error Example:](#)

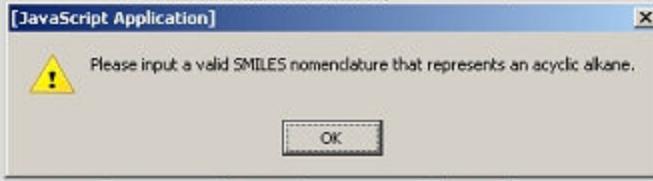
Topological Index Calculator

Select parent chain or ring

C1, methane

Bonds:

- Polarity: ?
- Weiner: ?
- Hosoya: ?
- Randic: ?
- Balaban: ?
- Harary: ?
- Vertex Degree Distance: ?



Compute

Clear Bonds

Add Data Line

SMILES: [?](#)

C1C(C)C(C(C)C)C(C)C1

Convert Edge List to SMILES

Compute using SMILES

Convert SMILES to Edge List

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Data:

Clear Console

Miscellaneous Tasks:

1. At any time, click Clear Bonds button to reset parent chain/ring, clear Bonds text field, clear SMILES

text field and clear index fields.

2. Click Add Data Line Button to allow entry of the boiling point of the molecule and transfer indices data to the Data Console.

The data in the data console can now be copied and pasted into a text file and saved as a .csv (comma separated value). Most spreadsheets can open this type of file. The data can be manipulated inside the spreadsheet for many indices.

Topological Index Calculator

Select parent chain or ring:
C5, pentane

Bonds:

1 2
2 3
3 4
4 5
2 6
4 7
3 8
8 9
8 10

[JavaScript Application] Please enter Boiling Point:
157.04
OK Cancel

Polarity: 12 ?
 Weiner: 117 ?
 Hosoya: 54 ?
 Randic: 4.4641 ?
 Balaban: 3.9835 ?
 Harary: 14.0833 ?
 Vertex Degree Distance: 5.8832 ?
 Odd-Even: 13.1667 ?

Compute Clear Bonds Add Data Line

SMILES: ?
Convert Edge List to SMILES
Compute using SMILES Convert SMILES to Edge List

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Data:

Clear Console

Topological Index Calculator

Select parent chain or ring:

C5, pentane

Bonds:

1 2
2 3
3 4
4 5
2 6
4 7
3 8
8 9
8 10

<input checked="" type="checkbox"/> Polarity:	12	?
<input checked="" type="checkbox"/> Weiner:	117	?
<input checked="" type="checkbox"/> Hosoya:	54	?
<input checked="" type="checkbox"/> Randic:	4.4641	?
<input checked="" type="checkbox"/> Balaban:	3.9835	?
<input checked="" type="checkbox"/> Harary:	14.0833	?
<input checked="" type="checkbox"/> Vertex Degree Distance:	5.8832	?
<input checked="" type="checkbox"/> Odd-Even:	13.1667	?

[Compute](#)

[Clear Bonds](#)

[Add Data Line](#)

SMILES: [?](#)

[Convert Edge List to SMILES](#)

[Compute using SMILES](#)

[Convert SMILES to Edge List](#)

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Data:

12, 117, 54, 4.4641, 3.9835, 14.0833, 5.8832, 13.1667, 157.04

[Clear Console](#)

- At any time click Clear Console button to clear the data console.