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A novel Lu index to QSPR studies of aldehydes and ketones

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A novel index based on the hyper-Wiener index, named Lu, was proposed. The relative bond length between two adjacent vertices in a molecular graph was taken into account in the definition of the Lu index. The usefulness of the new index in QSPR study was verified by its correlation with a number of organic compounds including aliphatic aldehydes and ketones. For each of the physical properties (the normal boiling points, molar refractions and gas heat capacities at 25°C), high quality QSPR models were obtained. The final models were validated to be statistically reliable using the leave-one-out cross validation and/or an external test set. The correlation coefficients (> 0.99) of all constructed models indicate the necessity of such an index, and show the potential of the Lu index for QSAR/QSPR studies.

KEY WORDS: Lu index, aldehydes, ketones, QSPR, physical properties

1. Introduction

A close relationship often exists between chemical structures of organic compounds and many of their physical and chemical properties and biological activities. It is very convenient for practical use and molecular design if the physicochemical properties or biological activities of a molecular can be calculated and predicted from its molecular structure. The quantitative structure–property/activity relationships (QSPR/QSAR) provide a powerful approach to this problem [1].

Mathematical descriptors derived from molecular graphs have been widely used in QSPR and QSAR which are known as topological indices. The hyper-Wiener index WW is one of the recently conceived distance-based graph invariants, used as a structural descriptor. The hyper-Wiener was introduced by Randić [2] and has been extensively studied. However, Randić's original

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definition of the hyper-Wiener index is applicable to trees only. Klein et al. [3] put forward that for both trees and cycle-containing structures.

$$\mathrm{WW}(G) = \frac{1}{2}\left[\Sigma d_{ij} + \Sigma d_{ij}^2\right], \tag{1}$$

where d_{ij} denotes the shortest path distance between vertices i and j in the graph G. The distance-related matrix used to calculate the hyper-Wiener index is made up of the shortest distances from a vertex i to all the other $(n-1)$ vertices in the molecular graphs, and the shortest distances of two adjacent atoms was regarded as "1". Although the Klein's graph-theory index has its advantage over the previous ones, it possesses a deficiency that it is not suitable for heteroatom-containing and multiple bond organic compounds.

The objective of the present work was to develop a novel index Lu based on the hyper-Wiener index, which can be used in heteroatom-containing and multiple bond containing organic compounds. The relative bond length between two adjacent vertices in a molecular graph was taken into account in the definition of the Lu index. The usefulness of the newly constructed index was verified by correlating with some properties of aldehydes and ketones.

2. Method

The *Lu* index is defined as follows:

$$\mathrm{Lu} = n^{1/2}\log\left[1/2(\Sigma D_{ij} + \Sigma D_{ij}^2)\right], \tag{2}$$

where n is the number of vertices in a molecular topological graph. D_{ij} is the shortest distance between vertices i and j, and is calculated by summing the relative bond length (take C–C bond length 0.154 nm as 1) [4] between two adjacent vertices in the shortest path.

The calculation of the Lu index was illustrated as following:

The shortest distance matrix D for the 2-butanone molecule is expressed as follows:

$$D = \begin{bmatrix} D_{11} & D_{12} & D_{13} & D_{14} & D_{15} \\ D_{21} & D_{22} & D_{23} & S_{24} & D_{25} \\ D_{31} & D_{32} & D_{33} & S_{34} & D_{35} \\ D_{41} & D_{42} & D_{43} & S_{44} & D_{45} \\ D_{51} & D_{52} & D_{53} & D_{54} & D_{55} \end{bmatrix} = \begin{bmatrix} 0 & 1 & 2 & 3 & 1.792 \\ 1 & 0 & 1 & 2 & 0.792 \\ 2 & 1 & 0 & 1 & 1.792 \\ 3 & 2 & 1 & 0 & 2.792 \\ 1.792 & 0.792 & 1.792 & 2.792 & 0 \end{bmatrix},$$

$$\mathrm{Lu} = n^{1/2}\log\left[1/2(\Sigma D_{ij} + \Sigma D_{ij}^2)\right] = 5^{1/2}\log(17.168 + 34.845) = 3.8373.$$

3. Result and discussion

3.1. Data set

The normal boiling points (BP) data are taken from Refs. [5–11]. Molar refractions (MR) data are taken from refs. [10–12]. The experimental values of gas heat capacity (C_p^G) are available in the literature [5].

3.2. Correlations to boiling points

We consider a mixed data set of 28 aldehydes and 60 ketones to develop the structure-boiling point model. The observed BP values are listed in table 1. The boiling point model is generated by using the Lu index and is expressed in equation (3).

$$\mathrm{BP} = -4.1047 + 20.3430\mathrm{Lu}, \tag{3}$$
$$R = 0.9953, \quad R_{\mathrm{cv}} = 0.9951, \quad s = 5.80, \quad s_{\mathrm{cv}} = 5.96, \quad F = 9236, \quad N = 88.$$

This model produces a standard error of 5.80 (°C) and explains more than 99.0% (R^2) of the variances in the experimental BP values for these compounds. On the other hand, the model is further validated using the leave-one-out cross-validation and an external test set, respectively. The R_{cv} and s_{cv} are determined to be 0.9951 and 5.96 (°C), which are very close to the statistics of equation (3). The cross-validation results demonstrate the model to be statistically significant. Furthermore, the model (Equation (3)) is used to predict the BP values of 16 compounds not involved in regression analysis. The predictive standard error s_{pred} is 3.63 (°C) for the test set, showing a good predictive power of the model.

It is should be noted that there are five compounds shown in table 1, nos. 8, 64, 74, and 85, 86 have larger errors than the twice of standard deviations. It is difficult to propose a reason for this and assess the reliability of data from different sources. However, if we discard these compounds, the quality of the model can be further improved. The standard error s for the remaining 83 compounds is significantly reduced to 4.96°C, which approximates the magnitude of experimental error.

The calculated BP values and Lu indices for 88 compounds are shown in table 1, and the experimental and predicted BP values for the 16 compounds are given in table 2.

As an extension of the above study, we deal with other application examples of this index. The MR and C_p^G of several data sets of compounds containing aldehydes and ketones are used in the following studies.

Table 1
Lu indices, calculated and experimental boiling points for aldehydes and ketones.

No.	Compound	Lu	BP (°C)		
			Exp	Cal.	Res
1	Acetaldehyde	1.6030	20.8	28.5	−7.7
2	Propionaldehyde	2.8631	48.8	54.1	−5.3
3	Butyl aldehyde	4.0566	75.7	78.4	−2.7
4	2-Methyl butanal	3.8296	64.4	73.8	−9.4
5	Pentaldehyde	5.2019	103.0	101.7	1.3
6	2-Methyl butanal	4.9177	92.5	95.9	−3.4
7	3-Methyl butanal	4.9942	92.5	97.4	−4.9
8	2,2-Dimethylpropanal	4.6903	77.5	91.3	−13.8
9	Hexanal	6.3083	128.0	124.2	3.8
10	2-Methylpentanal	6.0262	117.0	118.4	−1.4
11	3-Methylpentanal	6.0237	118.0	118.4	−0.4
12	2-Ethylbutanal	5.9143	117.0	116.2	0.8
13	Heptanal	7.3817	152.8	146.0	6.8
14	3-Methylhexanal	7.0797	143.0	139.9	3.1
15	2,2-Dimethylpentanal	6.7928	126.5	134.0	−7.5
16	Octanal	8.4261	171.0	167.3	3.7
17	2-Ethylhexanal	8.0192	160.0	159.0	1.0
18	2-Propylpentanal	7.9581	160.0	157.7	2.3
19	Nonanal	9.4447	191.0	188.0	3.0
20	3,5,5-Trimethylhexanal	8.7741	170.5	174.3	−3.8
21	Decanal	10.4402	208.5	208.2	0.3
22	Undecanal	11.4145	233.0	228.1	4.9
23	2-Methyldecanal	11.2360	229.0	224.4	4.6
24	Dodecanal	12.3694	254.0	247.5	6.5
25	2-Methylundecanal	12.2066	246.0	244.2	1.8
26	Tridecanal	13.3065	267.0	266.5	0.5
27	Tetradecanal	14.2270	287.0	285.3	1.7
28	Pentadecanal	15.1321	304.9	303.7	1.2
29	Acetone	2.6620	56.2	50.0	6.2
30	2-Butanone	3.8374	79.6	73.9	5.7
31	2-Pentanone	5.0022	102.0	97.6	4.5
32	3-Pentanone	4.9263	101.7	96.1	5.7
33	3-Methyl-2-butanone	4.7703	93.5	92.9	0.7
34	2-Hexanone	6.1327	127.6	120.6	7.0
35	3-Hexanone	6.0337	123.5	118.6	4.9
36	3-Methyl-2-pentanone	5.8227	118.0	114.3	3.7
37	4-Methyl-2-pentanone	5.9303	117.0	116.5	0.5
38	2-Methyl-3-pentanone	5.8258	115.5	114.4	1.2
39	3,3-Dimethyl-2-butanone	5.6035	106.0	109.8	−3.8
40	2-Heptanone	7.2279	151.4	142.9	8.5
41	3-Heptanone	7.1254	147.0	140.8	6.2
42	4-Heptanone	7.0893	144.0	140.1	3.0
43	3-Methyl-2-hexanone	6.9063	143.5	136.3	7.1
44	4-Methyl-2-hexanone	6.9396	139.0	137.0	1.9

Table 1
(*Continued*)

No.	Compound	Lu	BP (°C)		
			Exp	Cal.	Res
45	5-Methyl-2-hexanone	7.0534	144.0	139.3	4.6
46	2-Methyl-3-hexanone	6.9100	135.0	136.4	−1.4
47	4-Methyl-3-hexanone	6.8276	134.5	134.7	−0.3
48	5-Methyl-3hexanone	6.9431	135.0	137.1	−2.1
49	2,2-Dimethyl-3-pentanone	6.6353	125.6	130.8	−5.2
50	2,4-Dimethyl-3-pentanone	6.7105	125.4	132.4	−7.0
51	4,4-Dimethyl-3-pentanone	6.7553	126.4	133.3	−6.9
52	2-Octanone	8.2908	172.5	164.5	7.9
53	3-Octanone	8.1921	167.5	162.5	4.9
54	4-Octanone	8.1397	165.5	161.4	4.0
55	2-Methyl-4-heptanone	7.9801	154.0	158.2	−4.3
56	3-Methyl-4-heptanone	7.8683	153.0	155.9	−3.0
57	3-Methyl-2-heptanone	7.9822	164.0	158.2	5.7
58	6-Methyl-2-heptanone	8.1395	167.0	161.4	5.5
59	2-Methyl-3-heptanone	7.9858	158.0	158.3	−0.4
60	3,3-Dimethyl-2-hexanone	7.6364	151.5	151.2	0.2
61	2,2-Dimethyl-3-hexanone	7.7044	146.0	152.6	−6.6
62	2,5-Dimethyl-3-hexanone	7.8112	147.5	154.7	−7.3
63	4,4-Dimethyl-3-hexanone	7.5711	148.0	149.9	−1.9
64	2,2,4-Trimethyl-3-pentanone	7.5088	135.1	148.6	−13.6
65	2-Nonanone	9.3248	195.0	185.5	9.3
66	3-Nonanone	9.2323	190.0	183.7	6.2
67	4-Nonanone	9.1736	187.5	182.5	4.9
68	5-Nonanone	9.1534	188.4	182.1	6.2
69	7-Methyl-3-octanone	9.0940	182.5	180.8	1.5
70	3-Methyl-4-octanone	8.9105	174.0	177.1	−3.2
71	7-Methyl-4-octanone	9.0328	178.0	179.6	−1.7
72	2,6-Dimethyl-4-heptanone	8.8638	169.4	176.2	−6.9
73	3,5-Dimethyl-4-heptanone	8.6358	162.0	171.5	−9.6
74	2,2,4,4-Tetramethyl-3-pentanone	8.2986	152.0	164.7	−12.8
75	2-Decanone	10.3331	210.0	206.1	3.7
76	3-Decanone	10.2473	211.0	204.3	6.5
77	4-Decanone	10.1870	206.5	203.1	3.2
78	2-Undecanone	11.3182	231.5	226.1	5.2
79	3-Undecanone	11.2389	227.0	224.5	2.3
80	5-Undecanone	11.1427	227.0	222.5	4.2
81	6-Undecanone	11.1302	226.0	222.3	3.5
82	2-Dodecanone	12.2823	246.5	245.7	0.5
83	2-Tridecanone	13.2272	263.0	264.9	−2.3
84	7-Tridecanone	12.6150	261.0	260.9	8.2
85	2-Methyl-3-tridecanone	13.9645	267.0	279.9	−13.3
86	7-Ethyl-2-methyl-4-undecanone	13.4258	252.5	269.0	−16.8
87	2-Pentadecanone	15.0654	294.0	302.3	−8.8
88	8-Pentadecanone	14.8660	291.0	298.3	−7.7

Table 2
Lu indices, calculated and experimental boiling points for the test set of aldehydes and ketones.

No.	Compound	Lu	Test set BP (°C)		
			Exp	Cald	Res
1	4-Methylpentanal	6.1258	121.0	120.5	0.5
2	2-Methylhexanal	7.1192	141.0	140.7	0.3
3	4-Methylhexanal	7.1161	144.0	140.6	3.4
4	5-Methylhexanal	7.2222	143.5	142.8	0.7
5	4-Methyl-2-heptanone	7.9754	160.5	158.1	2.4
6	5-Methyl-3-heptanone	7.9206	161.0	157.0	4.0
7	3,5-Dimethyl-2-hexanone	7.8071	154.0	154.7	−0.7
8	4,5-Dimethyl-3-hexanone	7.6888	152.0	152.3	−0.3
9	3-Ethyl-4-methyl-2-pentanone	7.6139	154.0	150.7	3.3
10	4-Methyl-2-octanone	9.0095	184.0	179.1	4.9
11	2,5-Dimethyl-3-heptanone	8.7745	166.0	174.3	−8.3
12	3,3-Dimethyl-2-heptanone	8.6966	173.5	172.8	0.7
13	4,6-Dimethyl-3-heptanone	8.7502	171.5	173.9	−2.4
14	2,3-Dimethyl-4-heptanone	8.7093	167.5	173.0	−5.5
15	5-Decanone	10.1559	204.0	202.4	1.6
16	2,2,6,6-Tetramethyl-4-heptanone	9.6631	185.6	192.4	−6.8

3.3. Correlations to molar refraction

Molar refraction is a particularly useful physical parameter in chemistry, biological chemistry, and pharmaceutical science because it is closely related to the bulkiness and polarizability of a molecule. The compound dataset used in this study contains 22 aldehydes and 24 ketones. The compounds and the corresponding MR values are listed in table 3. The molar refraction model is constructed by using the Lu index and is obtained as follows:

$$\mathrm{MR} = 3.8169 + 4.3720\mathrm{Lu}, \tag{4}$$

$$R = 0.9976, \quad R_{\mathrm{cv}} = 0.9973, \quad s = 0.81, \quad s_{\mathrm{cv}} = 0.84, \quad F = 9002, \quad N = 46.$$

This model explains more than 99.5% of the variance in the experimental values of MR for 46 compounds. This model is validated to be statistically significant by the cross-validation. On the other hand, the best model (Equation (4)) is used to predict the MR values of five carbonyl compounds as the test set. The s_{pred} is 0.34 for the test set, indicating a good predictive power of the constructed model.

The calculated MR values and Lu indices for 46 compounds are shown in table 3, and the experimental and predicted MR values for the five compounds are given in table 4.

Table 3
Lu indices, calculated and experimental molar refractions for 46 compounds.

No.	Compound	Lu	MR ($cm^3\ mol^{-1}$)		
			Exp	Cald	Res
1	Acetaldehyde	1.6030	11.5829	10.8253	0.7576
2	Propionaldehyde	2.8631	16.1632	16.3345	−0.1713
3	Butyl aldehyde	4.0566	20.8011	21.5526	−0.7515
4	2-Methyl propanal	3.8296	20.8219	20.5601	0.2618
5	Pentaldehyde	5.2019	25.4983	26.5599	−1.0616
6	2-Methyl butanal	4.9177	25.3943	25.3173	0.0770
7	3-Methyl butanal	4.9942	25.5327	25.6518	−0.1191
8	Hexanal	6.3083	30.0928	31.3971	−1.3043
9	2-Methylpentanal	6.0262	29.8497	30.1638	−0.3141
10	2-Ethylbutanal	5.9143	29.9981	29.6745	0.3236
11	2,3-Dimethylbutanal	5.8167	30.0640	29.2478	0.8162
12	Heptanal	7.3817	34.7004	36.0901	−1.3897
13	2,2-Dimethylpentanal	6.7928	34.7537	33.5154	1.2383
14	Octanal	8.4261	39.4396	40.6562	−1.2166
15	2-Ethylhexanal	8.0192	39.2395	38.8772	0.3623
16	2-Ethyl-3-methylpentanal	7.7321	38.9423	37.6220	1.3203
17	Nonanal	9.4447	44.2669	45.1096	−0.8427
18	3,5,5-Trimethylhexanal	8.7741	43.9887	42.1777	1.8110
19	Decanal	10.4402	48.6737	49.4619	−0.7882
20	2-Methyldecanal	11.2360	53.0003	52.9412	0.0591
21	Dodecanal	12.3694	58.0913	57.8965	0.1948
22	2-Methyldecanal	12.2066	57.9284	57.1847	0.7437
23	Acetone	2.6620	16.2963	15.4553	0.8410
24	2-Butanone	3.8374	20.6039	20.5942	0.0097
25	2-Pentanone	5.0022	25.2926	25.6868	−0.3942
26	3-Pentanone	4.9263	25.2487	25.3549	−0.1062
27	3-Methyl-2-butanone	4.7703	25.2603	24.6729	0.5874
28	2-Hexanone	6.1327	29.9308	30.6294	−0.6986
29	3-Hexanone	6.0337	29.7251	30.1965	−0.4714
30	3-Methyl-2-pentanone	5.8227	29.9453	29.2740	0.6713
31	4-Methyl-2-pentanone	5.9303	29.9877	29.7445	0.2432
32	3,3-Dimethyl-2-butanone	5.6035	29.6748	28.3157	1.3591
33	2-Heptanone	7.2279	34.5463	35.4176	−0.8713
34	3-Heptanone	7.1254	34.4230	34.9695	−0.5465
35	4-Heptanone	7.0893	34.3083	34.8117	−0.5034
36	5-Methyl-2-hexanone	7.0534	34.5773	34.6547	−0.0774
37	2-Octanone	8.2908	39.1959	40.0647	−0.8688
38	5-Octanone	8.1397	39.0616	39.4041	−0.3425
39	6-Methyl-3-heptanone	8.0336	38.9478	38.9402	0.0076
40	2-Nonanone	9.3248	43.3542	44.5854	−1.2312
41	5-Nonanone	9.1534	43.8710	43.8360	0.0350

Table 3
(*Continued*)

No.	Compound	Lu	MR ($cm^3\ mol^{-1}$)		
			Exp	Cald	Res
42	2,6-Dimethyl-4-heptanone	8.8638	43.8902	42.5699	1.3203
43	2-Decanone	10.3331	48.5304	48.9937	−0.4633
44	2-Undecanone	11.3182	52.7129	53.3006	−0.5877
45	6-Undecanone	11.1302	53.2109	52.4787	0.7322
46	2-Methyl-4-undecanone	12.0165	57.7027	56.3536	1.3491

Table 4
Lu indices, calculated and experimental molar refractions for the test set of aldehydes and ketones.

No.	Compound	Lu	Test set		
			Exp	Cald	Res
1	2,2-Dimethylpropanal	4.6903	25.4202	24.3229	1.0973
2	3-Methylhexanal	7.0797	34.6622	34.7693	−0.1071
3	2,4-Dimethyl-3-pentanone	6.7105	34.1382	33.1552	0.9830
4	2-Methyl-3-hexanone	6.9100	34.5321	34.0274	0.5047
5	6-Methyl-2-heptanone	8.1395	39.4969	39.4028	0.0941

3.4. Correlations to gas heat capacity (C_p^G)

The gas heat capacity (C_p^G) is an important physical property of organic compounds for chemical engineering thermodynamics. Table 5 lists the experimental C_p^G data of 18 compounds, i.e., three aldehydes and 15 ketones. The gas heat capacity model is constructed by using the Lu index and is presented as follows:

$$C_p^G = 28.8049 + 21.4863\mathrm{Lu}, \tag{5}$$

$$R = 0.9978, \quad R_{\mathrm{cv}} = 0.9970, \quad s = 2.42, \quad s_{\mathrm{cv}} = 2.84, \quad F = 3696, \quad N = 18.$$

This model explains more than 99.2% of the variance in the experimental values of C_p^G for 18 compounds. This model is validated to be statistically significant by the cross-validation. The calculated C_p^G values and Lu indices for 18 compounds are shown in table 5.

According to Mihalić and Trinajstić's comments on the quality of model [13], the three constructed models all represent excellent QSPR models. Finally, it should be mentioned that the novel Lu index, which is based on the hyper-Wiener index, shows an excellent discrimination power of isomers for all investigated compounds in the database. Therefore, this index promises to be useful descriptor for QSPR/QSAR modeling in the future (figure 1).

Table 5
Lu indices, calculated and experimental gas heat capacities for aldehydes and ketones.

No.	Compound	Lu	C_p^G(J mol^{-1} K^{-1})		
			Exp	Cald	Res
1	Propionaldehyde	2.8631	90.03	90.32	−0.29
2	Pentaldehyde	5.2019	144.07	140.57	3.50
3	2,2-Dimethylpropanal	4.6903	132.42	129.58	2.84
4	Acetone	2.6620	83.99	86.00	−2.01
5	2-Butanone	3.8374	110.02	111.25	−1.23
6	2-Pentanone	5.0022	136.23	136.28	−0.05
7	3-Pentanone	4.9263	133.54	134.65	−1.11
8	3-Methyl-2-butanone	4.7703	131.09	131.30	−0.21
9	2-Hexanone	6.1327	161.50	160.57	0.93
10	3-Hexanone	6.0337	157.82	158.44	−0.62
11	4-Methyl-2pentanone	5.9303	155.68	156.22	−0.54
12	3,3-Dimethyl-2-butanone	5.6035	149.64	149.20	0.44
13	2-Heptanone	7.2279	189.55	184.10	5.45
14	4-Heptanone	7.0893	180.63	181.12	−0.49
15	2-Methyl-3-hexanone	6.9100	173.25	177.27	−4.02
16	2,4-Dimethyl-3-pentanone	6.7105	171.98	172.98	−1.00
17	2-Octanon	8.2908	209.54	206.94	2.60
18	5-Nonanone	9.1534	221.36	225.47	−4.11

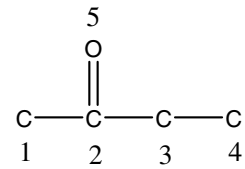

Figure 1. Description of skeletal structure of the 2-butanone molecule.

4. Conclusion

In this study, we define a novel topological index Lu by using the relative bond length of vertices. The usefulness of the newly constructed index was verified by its correlation with a number of organic compounds including aliphatic aldehydes and ketones. For each of the physical properties (the normal boiling points, molar refractions and gas heat capacities at 25°C), high quality QSPR models are obtained. In addition, the final models are validated to be statistically reliable using the leave-one-out cross validation and/or an external test set.

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