

Mean Molecular Radius and the Wiener Number: A Quest for Meaning

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The Wiener number (W) and its cubic root ($W^{1/3}$) were correlated with molecular radii (radius of gyration, s , and the mean molecular radius, r_m) of 14 homologous sets of straight-chain and branched alkanes, with 1–21 carbon atoms. From the linear regression equations of s , s^2 and s^3 on W , it can be concluded that the best results in terms of the correlation coefficient ($r^2 = 0.9906$ – 1.0000), as well as in terms of other regression parameters, were obtained with the response variable s^3 . This means that the Wiener number is most appropriately interpreted as molecular volume. Linear regression of s on $W^{1/3}$ gave similar results ($r^2 = 0.9885$ – 0.9994), suggesting $W^{1/3}$ should be interpreted as a molecular radius. The differences between the regression coefficient and regression parameters are more pronounced for less branched molecules. Analogous linear regressions of the mean molecular radius, r_m , differ little from the regressions of s .

Key words
Wiener number
mean molecular radius
radius of gyration
alkanes

INTRODUCTION

Since the appearance of Wiener's »path number« in 1947,¹ a curious fact that this simple topological index, based solely on molecular connectivity, can be successfully correlated with a great number of physical, chemical and biological parameters (from boiling points^{1–3} and gas-chromatographic retention data⁴ to stability constants of coordination compounds^{5–7} and biological activities^{8–10}) has led many scientists to a quest for its real physical meaning. The Wiener number (W) was claimed to reflect the size and shape of a molecule,¹¹ to be the measure of surface-to-volume ratio,¹² or to be intimately related to intermolecular forces.^{7,12,13} But, systematic analysis showed that the Wiener number is best correlated to the molecular surface area, and that it could be therefore most properly interpreted as a measure of this molecular quantity.¹⁴ Moreover, the authors plainly stated: » W is only weakly correlated to molecular volume of saturated hydrocarbons and does not reflect at all their surface-to-volume ratio. By this a long-existing

controversy concerning the physico-chemical interpretation of W is resolved.«¹⁴ This rather optimistic statement is based on the fact that the best correlation coefficients ($r = 0.858$ – 0.996) were obtained for the function $S_W = aW^{0.4} + b$, where S_W denotes the van der Waals surface of the molecule.

The impetus that moved me to question this statement was the observation that the Wiener number can be calculated from a mean (topological) square radius of a molecule^{15,16} and, on the other hand, that the Wiener number is fairly well correlated with its tridimensional counterpart (3-D Wiener number).¹⁷ Also, J. R. Platt found from the thermodynamic arguments that $W^{1/3}$ should be »a sort of a mean molecular diameter« or »a sort of mean distance between the carbon atoms«.¹⁸ Along these lines is also the definition of the mean (shortest-path) distance between vertices of an n -vertex graph, W/P (where $P = n(n-1)/2$ is the number of pairs of distinct sites in the graph), which makes $W \approx n^{2+1/d}$ (d is a dimension, possibly fractal), and therefore

the Wiener number should be interpreted as some sort of measure of linear extension.^{19–21} As the radius of gyration²² may be defined both as a kind of molecular radius (Eq. 2) and the root-mean-square distance between atoms (Eq. 3), in this paper I intend to find a correlation between this quantity (obtained by molecular-mechanics calculations) and the Wiener number.

METHODS

The Wiener number,^{2,23} $W = W(G)$, of a molecular graph G is defined as the half-sum of the elements of the distance matrix D of G :

$$W = (1/2) \sum_i \sum_j (D)_{ij} \quad (1)$$

where $(D)_{ij}$ represents the topological distance between vertices i and j in G .

The radius of gyration (s) is defined as the root-mean-square distance of atoms in a molecule from their common center of gravity:

$$s = [(n + 1)^{-1} \sum s_i^2]^{1/2} \quad (2)$$

where s_i denotes the distance of atom i from the center of gravity of the molecule in a specified conformation, and n is the number of atoms in the molecule. According to Lagrange's theorem, the radius of gyration can also be calculated from the Euclidean distance, r_{ij} , between all pairs i and j of atoms in a molecule:²²

$$s = [(n + 1)^{-2} \sum_i \sum_j r_{ij}^2]^{1/2} \quad (3)$$

The mean molecular radius (r_m) was calculated according to the formula:

$$r_m = n^{-1} \sum_i r_i \quad (4)$$

where r_i stands for the distance of the i -th atom from the geometrical center of the molecule. The geometrical center of the molecule is defined with Cartesian coordinates, x_i^c :

$$x_i^c = n^{-1} \sum_j x_{ji} \quad i = 1, 2, 3 \quad (5)$$

where x_{ji} denotes the i -th coordinate of the j -th atom.

The conformations of alkanes were generated by the computer program for molecular mechanics, developed by Kj. Rasmussen and co-workers,^{24–26} using the functions and parameters presented systematically elsewhere.²⁷ Radius of gyration (Eq. 3) and the mean molecular radius (Eq. 4) were calculated with a small computer programs, which I wrote specially for this purpose.

RESULTS

In order to find a correlation between the Wiener number and radii of a molecule, I generated 14 sets of structurally related alkanes, with 1–21 carbon atoms (Table I). The first three sets (Sets 1–3) consist of straight-chain alkane molecules in three general conformations (all- t ,

TABLE I. Sets of alkanes. N is the number of molecules in the set

Set	N	Number of atoms (C_n)	Number of atoms in the longest chain (C_m), conformation	Substituents	W	$B(G)^{(a)}$
1	13	C_1-C_{13}	C_1-C_{13}, t	–	0–364	0
2	9	C_5-C_{13}	C_5-C_{13}, tg	–	20–364	0
3	10	C_4-C_{13}	C_4-C_{13}, g	–	10–364	0
4	10	C_4-C_{14}	C_3-C_{13}, t	2-Me	9–444	2
5	11	C_5-C_{15}	C_3-C_{13}, t	2,2-diMe	16–526	3
6	10	C_7-C_{16}	C_4-C_{13}, t	2,2,3-triMe	42–603	5
7	10	C_8-C_{17}	C_4-C_{13}, t	2,2,3,3-tetraMe	58–674	6
8	10	C_8-C_{17}	C_4-C_{13}, t	$(m/2)$ - or $((m+1)/2)$ - <i>tert</i> -Bu	42–632	6
9	9	C_9-C_{17}	C_4-C_{12}, t	2-Me- $(m-1)$ - <i>tert</i> -Bu	170–886	8
10	11	C_4-C_{14}	C_3-C_{13}, t	$(m/2)$ - or $((m+1)/2)$ -Me	9–419	2
11	10	C_6-C_{16}	C_4-C_{14}, t	$(m/2)$ - or $((m+1)/2)$ -diMe	34–476	3
12	9	$C_{13}-C_{21}$	C_7-C_{15}, t	2,2-diMe- $(m/2+1)$ - or $((m+3)/2)$ - <i>tert</i> -Bu	253–1192	9
13	10	C_9-C_{18}	C_4-C_{13}, t	$(m/2)$ - or $((m+1)/2)$ -Me and <i>tert</i> -Bu	82–698	7
14	10	C_6-C_{15}	C_4-C_{13}, t	2, $(m-1)$ -diMe	29–538	4

^(a) Extent of branching $B(G)$ is defined as the sum of the number of branching points and the number of side chains in the graph of the molecule (Ref. 31).

TABLE II. Comparison of linear regressions from Tables S.I–S.VI (Supplement)

Variable		r^2	Slope		Intercept ^(a)		Ideal value ^(b)
Dp.	Ind.		Mean	Range	max / min	Mean	
s	W	0.9574	0.8619...0.9954	4.25	2.200	1.815...2.580	0.815
s^2	W	0.9895	0.9649...0.9990	3.13	3.866	3.224...4.572	0.664
s^3	W	0.9972	0.9906...1.0000	2.49	0.130	-9.304...6.161	0.541
s	$W^{1/3}$	0.9962	0.9885...0.9994	1.54	0.214	-0.376...0.839	0.815
s^2	$W^{1/3}$	0.9717	0.9427...0.9827	2.03	-10.059	-20.568...-2.631	0.664
s^3	$W^{1/3}$	0.9295	0.8591...0.9493	2.98	-75.94	-169.47...-21.38	0.541
r_m	W	0.9535	0.8514...0.9962	4.27	2.199	1.835...2.580	0.874
r_m^2	W	0.9866	0.9549...0.9991	3.15	4.123	3.355...4.950	0.764
r_m^3	W	0.9977	0.9937...0.9999	2.61	3.360	-3.463...7.874	0.668
r_m	$W^{1/3}$	0.9961	0.9857...0.9995	1.57	0.482	-0.416...1.064	0.874
r_m^2	$W^{1/3}$	0.9772	0.9551...0.9922	1.96	-7.211	-15.117...-1.254	0.764
r_m^3	$W^{1/3}$	0.9405	0.8798...0.9810	2.84	-55.05	-122.29...-14.63	0.668

^(a) All intercept values are given in the system of Ångstrom units (1 Å = 0.1 nm).

^(b) Values of s , s^2 , s^3 , r_m , r_m^2 , or r_m^3 for methane ($W = 0$).

all-*g*, *tgt*...), and the rest of the sets considered (3–14) consist of alkanes with various degrees of branching. All structures of branched alkanes were obtained by substitution of one to four hydrogen atoms in the parent straight-chain alkane molecule with methyl and/or *tert*-butyl group(s). In order to make a homologous series, the alkyl groups were substituted at the 2 and/or ($m-1$) position, or at the central position, $m/2$ or $(m+1)/2$, of the parent straight-chain alkane, C_mH_{2m+2} . Branched alkanes were generated from Set 1 of straight-chain alkanes, *i.e.*, they all had the same, all-*t*, conformation of the longest chain.

The calculated values of molecular radii s and r_m (Eqs. 3 and 4) for the molecules considered were correlated with their Wiener number (W) and its cube root ($W^{1/3}$). Also, I made linear regressions of the square and cube of the molecular radii (s^2 , s^3 , r_m^2 , r_m^3). Altogether 168 regression lines were obtained (see Supplement). All of them have a positive slope, and correlation coefficients vary between $r^2 = 0.8514$ and 1.0000.

DISCUSSION

By inspection of all 168 linear regressions (Table II) it is evident that the best regression coefficients, in terms of the mean value as well as their range, were obtained by the linear regression of s^3 (or r_m^3) on W and s (or r_m) on $W^{1/3}$. Thus, the Wiener number should be interpreted as a molecular volume ($\approx s^3$), and – accordingly – $W^{1/3}$ as a molecular radius. This is even more evident from the regression plots (Figures 1–3), which show that the low correlation is not caused by random scattering of data points, but rather by their curvilinear arrangement.

The notion that the Wiener number corresponds to the volume, and $W^{1/3}$ to the radius of the molecule is

even more evident from the analysis of the intercept and slope of the regression lines. Only the intercept values for regressions of s^3 (r_m^3) and s (r_m) on W and $W^{1/3}$, re-

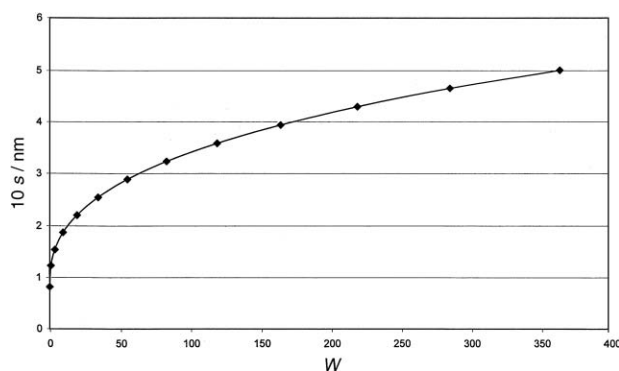


Figure 1. Plot of the radius of gyration, s , vs. the Wiener number, W , for 13 straight-chain alkanes in all-*t* conformation (Set 1, Table S.I, Supplement).

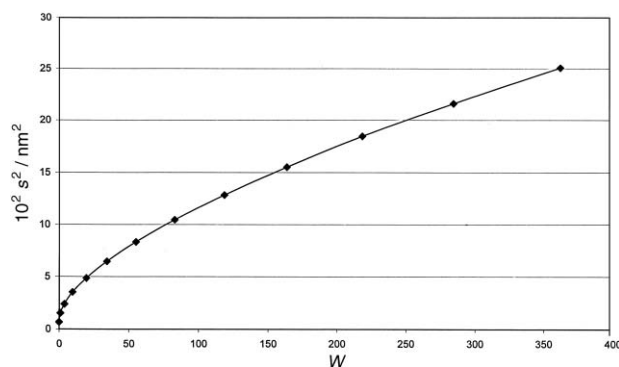


Figure 2. Plot of the square of the radius of gyration, s^2 , vs. the Wiener number, W , for 13 straight-chain alkanes in all-*t* conformation (Set 1, Table S.II, Supplement).

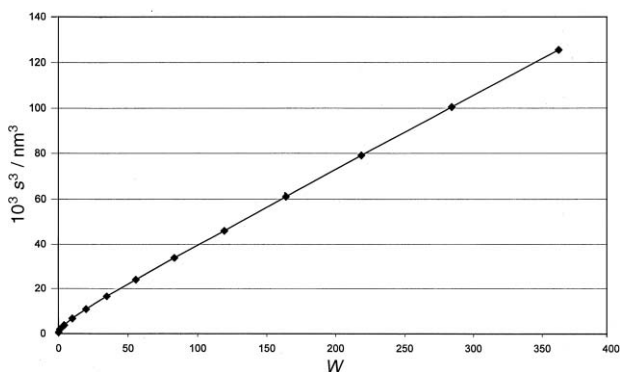


Figure 3. Plot of the cube of the radius of gyration, s^3 , vs. the Wiener number, W , for 13 straight-chain alkanes in all- t conformation (Set 1, Table S.III, Supplement).

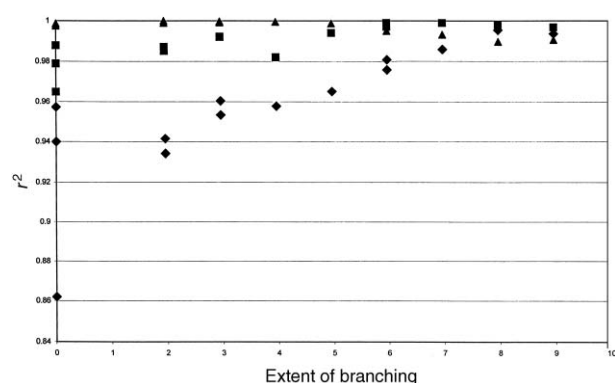


Figure 4. Dependence of the square of the correlation coefficient (r^2) on the extent of branching for the linear regressions of s (◆), s^2 (■), and s^3 (▲) on W (data from Tables S.III–S.V, Supplement). All the sets (1–14) of alkane molecules are included (Table I).

spectively, cover their ideal value (presented in Table II). Also, these regression lines have the smallest ratio of maximal and minimal slope values (1.54–2.61, Table II). Regressions on $W^{1/3}$ and W gave equally good results, but regressions on W seem to be slightly more successful. This stems from the mean values of r^2 (0.9962 vs. 0.9972 for s , 0.9961 vs. 0.9977 for r_m), mean intercept to its ideal value (0.214–0.815 vs. 0.130–0.541 for s , 0.482–0.874 vs. 3.360–0.668 for r_m) and the ratio of maximal and minimal slopes (1.54 vs. 2.49 for s , 1.57 vs. 2.61 for r_m). W is better correlated to r_m^3 than to s^3 , but the difference seems to be non-significant.

From the results presented it is evident that the correlation coefficients for regressions of s^3 on W ($r^2 = 0.9906$ – 1.0000) and s on $W^{1/3}$ ($r^2 = 0.9885$ – 0.9994) exceed fairly well the range of the best correlation coefficients of molecular surface (S_w) on W , as referred to in Gutman's paper¹⁴ ($r^2 = 0.736$ – 0.992). Therefore, as the most safe conclusion, W corresponds to the volume and $W^{1/3}$ to the length, but it is hardly possible to ascribe an intuitively clear meaning to this volume and length. In any case, s^3 is not a free or excluded molecular volume,

i.e., the quantities usually known as molecular volumes.^{28–30}

The thesis derived from the discussion that $W^{1/3}$ is a measure of molecular radius is not, however, without its shortcomings. First, the slope, as well as the intercept, of regression lines differs by even more than 10 of their standard errors, and depends not only on the constitution (slope = 4.964–6.367, Sets 1, 4–14, variable s , Table S.IV, Supplement) but also on the conformation of molecules (slope = 4.140–6.025, Sets 1–3, variable s , Table S.IV, Supplement). Therefore, $W^{1/3}$ is fairly well correlated with the molecular radius, but only for structurally and conformationally related molecules.

Analysis of the r^2 values shows that the interpretation of W as the molecular radius, area, or volume is also dependent on molecular constitution (Figure 4). For the straight-chain alkanes, the differences between r^2 values are prominent, but as the branching of chain progresses, linear regressions of s , s^2 and s^3 on W show virtually the same (very high) r^2 value. This means that, for very branched molecules, the Wiener number should also be interpreted as the molecular radius, molecular surface area, or molecular volume.

At the end of this discussion, I want to point to the fact that the Wiener number can be successfully correlated with many molecular properties; hence, neither the Wiener number, nor any quantity derived from it, should be identified with any molecular property. This is the first reason for the »mysterious« nature of the Wiener number and the other related topological indices.

Supplementary Materials. – Linear regression equations of molecular radii, the square of molecular radii and the cube of molecular radii on the Wiener number, W (Tables S.I–S.III) and on $W^{1/3}$ (Tables S.IV–S.VI) are prepared as the Supplement. These data are available via the Web under <http://pubwww.srce.hr/ccaca> or may be obtained from the author.

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SAŽETAK

Srednji molekularni radijus i Wienerov broj: u potrazi za značenjem

Nenad Raos

Wienerov broj (W) i njegov kubni korijen ($W^{1/3}$) korelirani su s molekularnim radijusima (radijusom vrtenja, s , i srednjim molekularnim radijusom, r_m) 14 homolognih skupova ravnih i razgrananih alkana s jednim do 21 ugljikovim atomom. Iz linearnih regresija s , s^2 i s^3 prema W može se zaključiti da se najbolji rezultati s obzirom na korelacijski koeficijent ($r^2 = 0,9906-1,0000$) i regresijske parametre dobivaju s varijablom s^3 . To znači da se Wienerov broj može najprikladnije interpretirati kao molekularni volumen. Linearna regresija s prema $W^{1/3}$ dala je slične rezultate ($r^2 = 0,9885-0,9994$), što navodi na to da bi $W^{1/3}$ trebalo shvatiti kao molekularni radijus. Razlike između regresijskog koeficijenta i regresijskih parametara to su izraženije što je molekula manje razgranana. Analogne linearne regresije prema srednjem molekularnom radijusu, r_m , malo se razlikuju od regresija prema s .

Mean Molecular Radius and the Wiener Number: A Quest for Meaning

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SUPPLEMENT

TABLE S.I. Linear regression equations of the molecular radii (s and r_m) on the Wiener number (W); S.E. is the standard error

Set	Dependent variable	10^4 Slope (S.E.) nm	10^1 Intercept (S.E.) nm	r^2
1	s	10.409 (1.256)	1.815 (0.196)	0.8619
1	r_m	8.940 (1.126)	1.835 (0.176)	0.8514
2	s	6.368 (0.508)	2.267 (0.095)	0.9573
2	r_m	5.400 (0.440)	2.263 (0.083)	0.9555
3	s	5.573 (0.498)	2.007 (0.089)	0.9399
3	r_m	4.714 (0.423)	2.053 (0.075)	0.9394
4	s	7.644 (0.676)	2.142 (0.143)	0.9342
4	r_m	6.509 (0.564)	2.159 (0.119)	0.9367
5	s	6.521 (0.480)	2.146 (0.123)	0.9534
5	r_m	5.620 (0.414)	2.157 (0.106)	0.9535
6	s	5.423 (0.365)	2.230 (0.112)	0.9651
6	r_m	4.650 (0.298)	2.241 (0.092)	0.9682
7	s	4.779 (0.236)	2.173 (0.084)	0.9808
7	r_m	4.079 (0.183)	2.200 (0.065)	0.9841
8	s	4.123 (0.229)	2.228 (0.077)	0.9759
8	r_m	3.429 (0.192)	2.259 (0.065)	0.9754
9	s	2.920 (0.075)	2.455 (0.039)	0.9954
9	r_m	2.911 (0.263)	2.168 (0.137)	0.9461
10	s	7.496 (0.623)	2.089 (0.124)	0.9415
10	r_m	6.257 (0.532)	2.119 (0.106)	0.9389
11	s	6.029 (0.433)	2.170 (0.105)	0.9604
11	r_m	4.965 (0.360)	2.183 (0.087)	0.9596
12	s	2.450 (0.075)	2.580 (0.054)	0.9936
12	r_m	2.094 (0.049)	2.580 (0.035)	0.9962
13	s	3.642 (0.154)	2.210 (0.059)	0.9859
13	r_m	2.936 (0.127)	2.267 (0.048)	0.9853
14	s	6.135 (0.455)	2.294 (0.125)	0.9578
14	r_m	5.292 (0.392)	2.296 (0.107)	0.9581

TABLE S.II. Linear regression equations of the square of molecular radii (s^2 and r_m^2) on the Wiener number (W); S.E. is the standard error

Set	Dependent variable	10^4 Slope (S.E.) nm ²	10^2 Intercept (S.E.) nm ²	r^2
1	s	6.565 (0.378)	3.233 (0.589)	0.9649
1	r_m	5.318 (0.348)	3.355 (0.544)	0.9549
2	s	4.228 (0.178)	4.572 (0.334)	0.9878
2	r_m	3.407 (0.160)	4.722 (0.302)	0.9846
3	s	3.189 (0.165)	3.743 (0.294)	0.9789
3	r_m	2.616 (0.148)	4.008 (0.264)	0.9750
4	s	5.394 (0.221)	3.914 (0.467)	0.9851
4	r_m	4.352 (0.192)	4.164 (0.406)	0.9828
5	s	4.708 (0.139)	3.689 (0.356)	0.9922
5	r_m	3.842 (0.128)	3.970 (0.327)	0.9902
6	s	4.064 (0.112)	3.678 (0.344)	0.9940
6	r_m	3.300 (0.093)	4.055 (0.287)	0.9937
7	s	3.576 (0.040)	3.224 (0.143)	0.9990
7	r_m	2.893 (0.031)	3.725 (0.109)	0.9991
8	s	2.870 (0.056)	4.001 (0.118)	0.9970
8	r_m	2.263 (0.054)	4.439 (0.184)	0.9954
9	s	2.296 (0.041)	4.332 (0.214)	0.9978
9	r_m	2.064 (0.147)	3.295 (0.597)	0.9789
10	s	5.085 (0.194)	3.729 (0.386)	0.9871
10	r_m	4.005 (0.179)	4.061 (0.357)	0.9824
11	s	4.201 (0.133)	3.787 (0.324)	0.9920
11	r_m	3.241 (0.120)	4.140 (0.293)	0.9891
12	s	2.097 (0.045)	4.337 (0.325)	0.9968
12	r_m	1.690 (0.002)	4.950 (0.156)	0.9989
13	s	2.556 (0.028)	3.743 (0.108)	0.9990
13	r_m	1.945 (0.032)	4.400 (0.122)	0.9978
14	s	4.634 (0.147)	4.137 (0.405)	0.9820
14	r_m	3.785 (0.134)	4.433 (0.367)	0.9901

TABLE S.III. Linear regression equations of the cube of molecular radii (s^3 and r_m^3) on the Wiener number (W); S.E. is the standard error

Set	Dependent variable	10^4 Slope (S.E.) nm ³	10^3 Intercept (S.E.) nm ³	r^2
1	s	3.409 (0.039)	3.425 (0.615)	0.9985
1	r_m	2.570 (0.054)	4.701 (0.842)	0.9952
2	s	2.166 (0.030)	6.161 (0.553)	0.9987
2	r_m	1.649 (0.029)	7.874 (0.541)	0.9979
3	s	1.410 (0.025)	5.576 (0.446)	0.9975
3	r_m	1.114 (0.029)	6.911 (0.518)	0.9946
4	s	3.016 (0.060)	2.286 (0.127)	1.0000
4	r_m	2.282 (0.015)	4.837 (0.321)	0.9996
5	s	2.683 (0.026)	0.009 (0.664)	0.9992
5	r_m	2.056 (0.075)	3.075 (0.191)	0.9999
6	s	2.378 (0.030)	-2.574 (0.936)	0.9987
6	r_m	1.814 (0.017)	1.549 (0.539)	0.9993
7	s	2.083 (0.052)	-5.209 (0.853)	0.9950
7	r_m	1.586 (0.035)	-0.322 (0.259)	0.9960
8	s	1.544 (0.023)	1.596 (0.771)	0.9983
8	r_m	1.146 (0.009)	5.283 (0.296)	0.9995
9	s	1.378 (0.053)	-3.157 (2.766)	0.9897
9	r_m	1.125 (0.034)	-3.463 (1.797)	0.9937
10	s	2.721 (0.029)	2.432 (0.572)	0.9990
10	r_m	2.001 (0.018)	5.241 (0.353)	0.9993
11	s	2.228 (0.013)	1.002 (0.323)	0.9997
11	r_m	1.633 (0.009)	4.526 (0.230)	0.9997
12	s	1.369 (0.034)	-9.304 (3.637)	0.9906
12	r_m	1.034 (0.032)	-1.414 (2.346)	0.9932
13	s	1.379 (0.027)	-0.231 (1.024)	0.9970
13	r_m	0.984 (0.015)	4.822 (0.397)	0.9995
14	s	2.738 (0.021)	-0.197 (0.574)	0.9995
14	r_m	2.102 (0.008)	3.417 (0.211)	0.9999

TABLE S.IV. Linear regression equations of molecular radii (s and r_m) on $W^{1/3}$; S.E. is the standard error

Set	Dependent variable	10^2 Slope (S.E.) nm	10^1 Intercept (S.E.) nm	r^2
1	s	6.025 (0.095)	0.631 (0.041)	0.9973
1	r_m	5.211 (0.045)	0.804 (0.020)	0.9992
2	s	5.115 (0.098)	0.770 (0.050)	0.9974
2	r_m	4.343 (0.072)	0.932 (0.037)	0.9981
3	s	4.140 (0.045)	0.839 (0.022)	0.9991
3	r_m	3.503 (0.034)	1.064 (0.017)	0.9992
4	s	6.267 (0.087)	0.320 (0.045)	0.9983
4	r_m	5.329 (0.069)	0.611 (0.036)	0.9985
5	s	6.180 (0.124)	0.165 (0.069)	0.9982
5	r_m	5.326 (0.010)	0.449 (0.057)	0.9966
6	s	6.271 (0.110)	-0.116 (0.067)	0.9975
6	r_m	5.367 (0.106)	0.236 (0.065)	0.9969
7	s	6.085 (0.156)	-0.238 (0.102)	0.9973
7	r_m	5.179 (0.155)	0.151 (0.100)	0.9929
8	s	4.964 (0.144)	0.317 (0.092)	0.9934
8	r_m	4.130 (0.114)	0.688 (0.073)	0.9939
9	s	5.130 (0.209)	-0.044 (0.160)	0.9885
9	r_m	5.237 (0.238)	-0.416 (0.182)	0.9857
10	s	5.930 (0.114)	0.388 (0.058)	0.9967
10	r_m	4.960 (0.068)	0.694 (0.034)	0.9983
11	s	5.910 (0.052)	0.148 (0.029)	0.9994
11	r_m	4.870 (0.040)	0.516 (0.023)	0.9995
12	s	5.388 (0.202)	-0.376 (0.173)	0.9903
12	r_m	4.599 (0.166)	0.058 (0.142)	0.9909
13	s	4.996 (0.125)	0.120 (0.084)	0.9950
13	r_m	4.030 (0.096)	0.575 (0.065)	0.9977
14	s	6.367 (0.086)	0.074 (0.050)	0.9985
14	r_m	5.492 (0.076)	0.381 (0.045)	0.9985

TABLE S.V. Linear regression equations of the square of molecular radii (s^2 and r_m^2) on $W^{1/3}$; S.E. is the standard error

Set	Dependent variable	10^4 Slope (S.E.) nm ²	10^2 Intercept (S.E.) nm ²	r^2
1	s	3.492 (0.260)	-3.066 (1.127)	0.9427
1	r_m	2.862 (0.187)	-1.873 (0.813)	0.9551
2	s	3.316 (0.173)	-5.436 (0.888)	0.9813
2	r_m	2.681 (0.123)	-3.391 (0.632)	0.9854
3	s	2.302 (0.107)	-2.631 (0.530)	0.9827
3	r_m	1.896 (0.079)	-1.254 (0.390)	0.9862
4	s	4.248 (0.244)	-8.098 (1.257)	0.9712
4	r_m	3.437 (0.185)	-5.575 (0.954)	0.9746
5	s	4.307 (0.269)	-9.795 (1.498)	0.9661
5	r_m	3.526 (0.206)	-7.092 (1.146)	0.9702
6	s	4.583 (0.249)	-13.210 (1.520)	0.9770
6	r_m	3.723 (0.198)	-9.671 (1.212)	0.9778
7	s	4.452 (0.283)	-14.184 (1.828)	0.9688
7	r_m	3.600 (0.230)	-10.350 (1.488)	0.9684
8	s	3.375 (0.217)	-8.804 (1.385)	0.9680
8	r_m	2.670 (0.158)	-5.712 (1.009)	0.9728
9	s	3.990 (0.266)	-14.991 (2.032)	0.9698
9	r_m	3.663 (0.123)	-14.649 (0.939)	0.9922
10	s	3.870 (0.236)	-7.804 (1.196)	0.9675
10	r_m	3.069 (0.160)	-4.556 (0.813)	0.9760
11	s	4.019 (0.189)	-9.761 (1.060)	0.9827
11	r_m	3.111 (0.129)	-6.369 (0.725)	0.9864
12	s	4.564 (0.284)	-20.568 (2.440)	0.9735
12	r_m	3.678 (0.222)	-15.117 (1.901)	0.9752
13	s	3.448 (0.193)	-10.600 (1.297)	0.9755
13	r_m	2.632 (0.133)	-6.656 (0.892)	0.9801
14	s	4.675 (0.253)	-11.872 (1.477)	0.9770
14	r_m	3.827 (0.194)	-8.695 (1.130)	0.9799

TABLE S.VI. Linear regression equations of the cube of molecular radii (s^3 and r_m^3) on $W^{1/3}$; S.E. is the standard error

Set	Dependent variable	10^2 Slope (S.E.) nm ³	10^2 Intercept (S.E.) nm ³	r^2
1	s	1.701 (0.208)	-2.506 (0.902)	0.8591
1	r_m	1.300 (0.145)	-1.744 (0.629)	0.8798
2	s	1.661 (0.145)	-4.327 (0.745)	0.9493
2	r_m	1.272 (0.099)	-3.011 (0.508)	0.9594
3	s	0.9916 (0.0806)	-2.138 (0.396)	0.9498
3	r_m	0.7886 (0.0572)	-1.463 (0.281)	0.9596
4	s	2.293 (0.227)	-6.008 (1.173)	0.9186
4	r_m	1.744 (0.161)	-4.344 (0.829)	0.9290
5	s	2.378 (0.244)	-7.283 (1.357)	0.9136
5	r_m	1.832 (0.175)	-5.325 (0.974)	0.9241
6	s	2.619 (0.239)	-9.712 (1.461)	0.9375
6	r_m	2.004 (0.174)	-7.139 (0.107)	0.9428
7	s	2.540 (0.254)	-10.329 (1.644)	0.9259
7	r_m	1.937 (0.188)	-7.519 (1.217)	0.9298
8	s	1.776 (0.175)	-6.487 (1.115)	0.9283
8	r_m	1.326 (0.119)	-4.453 (0.759)	0.9396
9	s	2.370 (0.222)	-11.725 (1.695)	0.9421
9	r_m	1.970 (0.103)	-9.926 (0.790)	0.9810
10	s	2.002 (0.204)	-5.214 (1.031)	0.9149
10	r_m	1.487 (0.132)	-3.560 (0.670)	0.9336
11	s	2.130 (0.179)	-6.980 (1.008)	0.9463
11	r_m	1.535 (1.147)	-4.670 (0.644)	0.9573
12	s	2.951 (0.259)	-16.947 (2.220)	0.9489
12	r_m	2.238 (0.189)	-12.292 (1.625)	0.9523
13	s	1.831 (0.158)	-7.569 (1.064)	0.9435
13	r_m	1.314 (0.100)	-4.948 (0.677)	0.9352
14	s	2.692 (0.251)	-9.086 (1.461)	0.9352
14	r_m	2.076 (0.179)	-6.670 (1.045)	0.9437