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Abstract

Motivation. The eigenvalue of bonding orbital–connecting matrix is a good descriptor for expressing the relative bond energies of C–C and C–H bonds in alkanes. This approach should be extended to QSPR for other properties and other compounds besides alkanes. In this paper we investigate the correlation between the eigenvalue of bonding orbital–connecting matrix and the density of monoderivative of hydrocarbon.

Method. Multivariable models were developed to predict the densities of alkanes and monosubstituted alkanes based on the eigenvalues of bonding orbital–connecting matrix, polarizability effect index (PEI) of alkyl, and Pauling's electronegativity. These compounds are of special interest to petroleum or chemical engineers. The densities of monosubstituted alkanes RX (X = NH_2, OH, SH, F, Cl, Br, I) and alkanes can be correlated by a simple QSPR expression.

Results. Using these QSPR models to estimate the densities for RX, the root–mean–square error (rms), the average absolute error and the average relative error between the experimental and estimated values are only 0.0208 g/cm^3, 0.0171 g/cm^3 and 1.85%, respectively.

Conclusions. Not only can the models of this paper give precise calculated results but also they have good predictive ability. The models can be used to predict the densities of alkanes and monosubstituted alkanes whose densities are not yet experimentally measured.

Keywords. Polarizability effect index PEI; bonding orbital–connecting matrix; molar volume; density; monoderivative of hydrocarbon; alkane.

1 INTRODUCTION

The density of organic compounds (especially the densities of alkanes and monosubstituted alkanes) is an important physical property for selecting production facilities in the chemical and petrochemical industries. For example, the density, one of the major physiochemical properties, is frequently utilized in material accounting and transfer procedure by engineers, and is also used to characterize and identify a compound. In addition, density can be used to predict or estimate other

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physical properties (such as critical pressures) of organic compounds [1,2]. Unfortunately, compilations of the experimentally derived density values may not be available for all organic compounds of interest. In many cases, it is impractical or impossible to measure the property of the interested compound because insufficient material exists to be tested, there are toxicity issues, or the number of compounds for which data are needed is very large. Thus a reliable means of estimating density for engineers would be an advantage. Up to now, only few methods originating from the molecular structure of organic compound have been proposed for estimating density [2,3,4]. Karelson [2] and co–workers calculated the molar volume for liquid organic compound by semi–empirical AM1 and then converted the molar volume to density, which gives their model an intrinsic mean of density. Liu [3,4] used neural networks to predict the densities for alkanes.

This paper focuses on the practical and rational model for evaluating the density of organic compound, which depends on the chemical environment of molecular bonds.

2 MATERIALS AND METHODS

At a specific temperature, the density of a compound can be expressed as:

$$D = M/V \tag{1}$$

were M is the molar mass and V denotes the molar volume. We consider that for an alkane RH the molar volume V_{RH} can be mainly divided into two parts: (*i*) the contributions of C–C bonds and (*ii*) the contributions of C–H bonds. That is,

$$V_{RH} = a_0 + b_0 \Sigma V_{C-C} + c_0 \Sigma V_{C-H} \tag{2}$$

The $V_{C–C}$ and $V_{C–H}$ are the contributions of per molar C–C and per molar C–H bond to the molar volume, respectively. Roughly, if the volume of a C–C bond or a C–H bond can be regarded as a constant, the molar volume of the alkane may be proportional to the numbers of C–C and C–H bonds. In facts, since the chemical environment of the C–C bonds in the alkane is different from each other, their volume is not a constant. Therefore, taking the simple additivity of the number of the C–C bond in the alkane as its volume contribution directly will raise a large estimating error. So do for the C–H bonds. Our recent research result [5,6] shows that not only the chemical environment, but also the bond energies of the C–C and C–H bonds can be distinguished and characterized well by the eigenvalues X_{1CC} and X_{1CH} of C–C and C–H bond orbital–connecting matrices, respectively. For a same kind of chemical bond, say C–C or C–H bond, it is presumed that the stronger the bond energy is, the shorter the bond length will be, and the smaller the volume contribution will be. Thus, it can be leaded to the expressions, $V_{C–C} = kX_{1CC}$ and $V_{C–H} = mX_{1CH}$. Replacing $V_{C–C}$ and $V_{C–H}$ with kX_{1CC} and mX_{1CH} in Eq. (2), we get

$$V_{RH} = a_0 + b_0 \Sigma(kX_{1CC}) + c_0 \Sigma(mX_{1CH}) = a + b\Sigma X_{1CC} + c\Sigma X_{1CH} \tag{3}$$

Where, X_{1CC} and X_{1CH} are the eigenvalues of C–C and C–H bond orbital–connecting matrices, respectively, *a*, *b* and *c* are the regression coefficients that can be got by least–square fitting of the eigenvalues to the experimental data of the molar volume V_{RH} ($V_{RH} = M_{RH}/D_{RH}$, here the M_{RH} and D_{RH} are molar mass and density of the alkane). Combining Eq. (1) and Eq. (3), we get

$$D_{RH} = \frac{M_{RH}}{a + b\Sigma X_{1CC} + c\Sigma X_{1CH}} \tag{4}$$

The above equation is expected to estimate the densities of alkanes.

2.1 Polarizability Effect Index (PEI) of Alkyl R

Firstly, by cutting down a C_i–C_j or a C_i–H bond of a given alkane molecule, one gets two alkyls R_i and R_j. The calculation of PEI had been elaborated in literature [7]. According to the literature [7], the PEI values of alkyl R_i and R_j can be calculated easily. Here, for the convenience, the PEI values of some normal alkyls and the increments ΔPEI are cited in Table 1.

Table 1. The PEI and ΔPEI values of normal alkyl $H(CH_2)_N$

N	PEI	ΔPEI	*N*	PEI	ΔPEI
1	1.0000	1.0000	6	1.2350	0.0095
2	1.1405	0.1405	7	1.2414	0.0064
3	1.1887	0.0481	8	1.2461	0.0047
4	1.2122	0.0235	9	1.2498	0.0037
5	1.2260	0.0138	10	1.2527	0.0029

2.2 C–C and C–H σ Bonds Orbital–Connecting Matrices and Their Eigenvalues

For the convenience of readers, here the calculation of parameters of ΣX_{1CC} and ΣX_{1CH} [5,6] for σ bonds were restated briefly. Firstly, using the polarizability effect index PEI(R_i) and PEI(R_j) of the alkyls as the main–diagonal element, 1 as the off–diagonal element, it can be constructed the orbital–connecting matrix $CM_{ij,m}$ for C_i–C_j σ bond, and using PEI(R_i), PEI(H) as the main–diagonal element, 1 as the off–diagonal element, it can be constructed the orbital–connecting matrix $CM_{i\mathrm{H},m}$ for C_i–H σ bond, respectively. Then solving the matrices, two eigenvalues for each $CM_{ij,m}$ or $CM_{i\mathrm{H},m}$ was got, and the smaller one of each pair of eigenvalues was assigned as X_{1CC} and X_{1CH} respectively. Finally, the parameters ΣX_{1CC} and ΣX_{1CH} were obtained by summing up all X_{1CC} and X_{1CH} of the C_i–C_j and C_i–H bonds in an alkane molecule.

Consider 2–methylbutane as an example to compute the parameters ΣX_{1CC} and ΣX_{1CH}. The calculation procedures of ΣX_{1CC} and ΣX_{1CH} are listed in Table 2 and Table 3, respectively.

Table 2. Calculation of ΣX_{1CC} for 2–methylbutane

C_i–C_j bond	R_i PEI(R_i)	R_j PEI(R_j)	$CM_{ij,m}$	X_{1CC} (the smaller eigenvalue)	Wt [a]
CH_3—$CH_2CH(CH_3)_2$	CH_3• 1.0000	• $CH_2CH(CH_3)_2$ 1.2368	$\begin{bmatrix} 1.0000 & 1 \\ 1 & 1.2368 \end{bmatrix}$	0.1114	1
CH_3CH_2—$CH(CH_3)_2$	CH_3CH_2• 1.1405	•$CH(CH_3)_2$ 1.2810	$\begin{bmatrix} 1.1405 & 1 \\ 1 & 1.2810 \end{bmatrix}$	0.2083	1
$CH_3CH_2CH(CH_3)$–CH_3	$CH_3CH_2\dot{C}HCH_3$ 1.3292	•CH_3 1.0000	$\begin{bmatrix} 1.3292 & 1 \\ 1 & 1.0000 \end{bmatrix}$	0.1511	2

ΣX_{1CC}= 0.1114+0.2083+0.1511+0.1511=0.6219

[a] Wt denotes the number of a sort of C–C bond in the compound

Table 3. Calculation of ΣX_{1CH} for 2–methylbutane

C_i–H bond	R_i PEI(R_i)	H PEI(H)	$CM_{iH,m}$	X_{1CH}(the smaller eigenvalue)	Wt [a]
$CH_3CH_2CH(CH_3)CH_2$–H	$CH_3CH_2CH(CH_3)CH_2$• 1.2603	• H 0	$\begin{bmatrix} 1.2603 & 1 \\ 1 & 0 \end{bmatrix}$	–0.5518	6
$CH_3CH_2(CH_3)_2C$—H	$CH_3CH_2\dot{C}(CH_3)_2$ 1.4697	• H 0	$\begin{bmatrix} 1.4697 & 1 \\ 1 & 0 \end{bmatrix}$	–0.5061	1
H–$CH(CH_3)CH(CH_3)_2$	$CH_3\dot{C}HCH(CH_3)_2$ 1.3773	• H 0	$\begin{bmatrix} 1.3773 & 1 \\ 1 & 0 \end{bmatrix}$	–0.5255	2
H–$CH_2CH_2CH(CH_3)_2$	• $CH_2CH_2CH(CH_3)_2$ 1.2357	• H 0	$\begin{bmatrix} 1.2357 & 1 \\ 1 & 0 \end{bmatrix}$	–0.5576	3

ΣX_{1CH}= –0.5518×6+(–0.5061)+(–0.5255) ×2+(–0.5576) ×3=–6.5407

[a] Wt denotes the number of a sort of C–H bond in the compound.

Likewise, all the ΣX_{1CC}, ΣX_{1CH} values of alkanes were calculated and listed in Table 4.

2.3 Regression Analysis

Experimental densities (at 1 atm and 25 ^oC) data [8] are available for 94 alkanes and presented in Table 4. The predictive ability of the obtained equations in the text was examined by the leave–one–out (LOO) cross–validation method. Taking experimental densities D_{RH} (at 1 atm and 25 ^oC) of 94 alkanes as data set, using Eq. (4) as the model, we obtained Eq. (5).

$$D_{RH} = \frac{M_{RH}}{4.4823 - 12.6316\Sigma X_{1CC} - 18.6198\Sigma X_{1CH}} \quad (5)$$

$$n = 94 \quad R{=}0.998 \quad R^2_A = 0.993 \quad \mathrm{F} = 2722.60 \quad SEE = 0.0107$$
$$PRESS = 0.0117 \quad SSY = 49.738 \quad R^2_{CV} = 0.99 \quad S_{PRESS} = 0.0113 \quad PSE = 0.0112$$

The correlation coefficient 0.998 shows Eq. (5) a good correlation. From the statistics of LOO cross–validation, it can be seen that Eq. (5) has a good predictive ability and good stability. Thus Eq. (5) is recommended to predict the densities of alkanes. The estimated and predicted densities of alkanes by Eq. (5) are listed in Table 4 and Table 6 respectively.

3 RESULTS AND DISCUSSION

The densities of alkanes can be estimated well by Eq. (5), and we want to find if the densities of monosubsituted alkanes can also be estimated by a similar equation. When a hydrogen atom in the alkane RH is replaced by a substituent X (X designated halogen or other functional groups), the monosubstituted alkane molecule RX will generate. Compared the two series of compounds, it can be found there are two primary discrepancy between compounds RH and RX: (*i*) A C–H bond in alkane has changed into the corresponding C–X bond; (*ii*) Generally speaking, the alkane molecule RH is nonpolar, while RX belongs to the polar molecule. If taking the alkane RH as the unperturbed system and the monosubstituted alkane RX as the corresponding perturbed system, one can, based on the unperturbed system, estimate the molar volume V_{RX} for the perturbed system RX with Eq. (6).

$$V_{RX} = V_{RH} + \Delta\Delta V + V_X \tag{6}$$

where V_{RH} is the molar volume of the unperturbed system RH; $\Delta\Delta V$ designates the volume increments of the alkyl R from RH system to RX system, which is caused by the H atom changing into the substituent X; V_X is the molar volume of the substituent X, which, we suppose, can be scaled approximately by the atomic radii (r_X) of the atom attached directly to the alkyl R. The volume increments $\Delta\Delta V$ is the difference between the volume of alkyl R in the RH and that in the RX respectively, which, we think, can be correlated with the polarizability of the alkyl R and the electronegativity of the group X. Based on the above analysis, we suggest a single expression, Eq. (7), to evaluate the densities for different series of monosubstituted alkanes RX.

$$D_{RX} = \frac{M_{RX}}{a + br_X + cPEI + dPEI \times \chi_X + e\Sigma X_{1CC} + f\Sigma X_{1CH}} \tag{7}$$

where M_{RX} and D_{RX} are molar mass and density of the compound RX respectively. The r_x and χ_x are the atomic radii [9] and electronegativity (Pauling scale) of the atom attached directly to the alkyl R, respectively. PEI is the polarizability effect index of the alkyl R in RX. ΣX_{1CC} and ΣX_{1CH} is the sum of eigenvalues of matrices $CM_{ij,m}$ and $CM_{iH,m}$ for C–C and C–H bonds in the alkyl R, respectively.

Now, take 2–bromo–2–methylbutane for example to show the calculation of ΣX_{1CC} and ΣX_{1CH} for RX. At first, the bromine atom was replaced with a hydrogen atom, that is, $(CH_3)_2CBrCH_2CH_3$ was returned to $(CH_3)_2CHCH_2CH_3$. Then the bonding orbital–connecting matrices $CM_{ij,m}$ and $CM_{iH,m}$ were constructed as the treatment of 2–methylbutane (see Table 2 and Table 3), and the X_{1CC} and X_{1CH} values, 0.6219 and –6.5407 were obtained, respectively. Since having the same σ carbon–carbon bond skeleton, the 2–bromo–2–methylbutane $(CH_3)_2CBrCH_2CH_3$ has the equal ΣX_{1CC} value as that of the 2–methylbutane $(CH_3)_2CHCH_2CH_3$, that is, its ΣX_{1CC}=0.6219. Comparing with $(CH_3)_2CHCH_2CH_3$, 2–bromo–2–methylbutane $(CH_3)_2CBrCH_2CH_3$ loses one C–H

bond which is the bond $Et(Me)_2C–H$, therefore its ΣX_{1CH} value must be cut out the X_{1CH} value of the lost C–H bond. That is, its ΣX_{1CH}=(–0.5518×6+(–0.5061)+(–0.5255)×2+(–0.5576)×3) – (–0.5061) = –6.5407–(–0.5061) =–6.0346. Likewise, all the parameter values of ΣX_{1CC}, ΣX_{1CH} for monosubstituted alkanes were calculated and listed in Table 5.

Table 4. Experimental density values (at 1 atm and 25 °C) for 94 alkanes

No	RH	ΣX_{1CC}	ΣX_{1CH}	$D_{exp.}$ (g/cm^3)	D_{calc} [a] (g/cm^3)	Δ [b]
1	propane	0.1356	–4.5074	0.4930	0.5075	–0.0145
2	butane	0.3203	–5.5244	0.5730	0.5615	0.0115
3	2–methyl–propane	0.3921	–5.5327	0.5510	0.5656	–0.0146
4	2,2–dimethyl–propane	0.7552	–6.5532	0.5852	0.6156	–0.0304
5	hexane	0.7533	–7.5404	0.6548	0.6353	0.0195
6	2–methyl–pentane	0.8540	–7.5453	0.6500	0.6409	0.0091
7	3–methyl–pentane	0.8753	–7.5440	0.6598	0.6423	0.0175
8	2,2–dimethyl–butane	1.0264	–7.5706	0.6444	0.6492	–0.0048
9	octane	1.2266	–9.5424	0.6986	0.6840	0.0146
10	2,3–dimethyl–hexane	1.4990	–9.5407	0.6912	0.6986	–0.0074
11	2,4–dimethyl–hexane	1.4798	–9.5432	0.6962	0.6973	–0.0011
12	2,5–dimethyl–hexane	1.4418	–9.5482	0.6901	0.6949	–0.0048
13	3,4–dimethyl–hexane	1.5284	–9.5370	0.7151	0.7004	0.0147
14	2,2,4–trimethyl–pentane	1.6445	–9.5487	0.6877	0.7059	–0.0182
15	2–methyl–octane	1.5800	–10.5423	0.7095	0.7079	0.0016
16	3–methyl–octane	1.6165	–10.5373	0.7170	0.7101	0.0069
17	4–methyl–octane	1.6299	–10.5432	0.7160	0.7103	0.0057
18	2,4–dimethyl–heptane	1.7439	–10.5347	0.7115	0.7167	–0.0052
19	3–ethyl–heptane	1.6668	–10.5296	0.7225	0.7131	0.0094
20	4–ethyl–heptane	1.6803	–10.5265	0.7241	0.7141	0.0100
21	2,2,3–trimethyl–hexane	1.9732	–10.5326	0.7257	0.7286	–0.0029
22	2,3,3–trimethyl–hexane	2.0003	–10.5284	0.7345	0.7304	0.0041
23	2,3,4–trimethyl–hexane	1.9256	–10.5280	0.7354	0.7265	0.0089
24	2,4,4–trimethyl–hexane	1.9640	–10.5333	0.7201	0.7281	–0.0080
25	3,3,4–trimethyl–hexane	2.0291	–10.5253	0.7414	0.7321	0.0093
26	2–methyl–4–ethyl–hexane	1.7826	–10.5409	0.7195	0.7182	0.0013
27	3–methyl–3–ethyl–hexane	1.9151	–10.5239	0.7371	0.7263	0.0108
28	2,2,3,3–tetramethyl–pentane	2.2165	–10.5260	0.7530	0.7421	0.0109
29	2,3–dimethyl–3–ethyl–pentane	2.0373	–10.5208	0.7508	0.7329	0.0179
30	2,2–dimethyl–octane	2.0324	–11.5370	0.7208	0.7334	–0.0126
31	2,4–dimethyl–octane	2.0018	–11.5368	0.7226	0.7319	–0.0093
32	2,5–dimethyl–octane	1.9952	–11.5282	0.7264	0.7322	–0.0058
33	2,7–dimethyl–octane	1.9391	–11.5382	0.7202	0.7289	–0.0087
34	3,3–dimethyl–octane	2.1024	–11.5263	0.7351	0.7375	–0.0024
35	3,4–dimethyl–octane	2.0581	–11.5196	0.7410	0.7358	0.0052
36	3,5–dimethyl–octane	2.0393	–11.5221	0.7329	0.7348	–0.0019
37	3,6–dimethyl–octane	2.0185	–11.5266	0.7324	0.7334	–0.0010
38	4,4–dimethyl–octane	2.1275	–11.5196	0.7312	0.7392	–0.0080
39	4,5–dimethyl–octane	2.0709	–11.5168	0.7432	0.7367	0.0065
40	3–ethyl–octane	1.9220	–11.5227	0.7359	0.7291	0.0068
41	4–ethyl–octane	1.9423	–11.5178	0.7343	0.7304	0.0039
42	2,2,3–trimethylheptane	2.2363	–11.5382	0.7385	0.7432	–0.0047
43	2,2,4–trimethylheptane	2.2090	–11.5255	0.7237	0.7427	–0.0190
44	2,2,5–trimethylheptane	2.1848	–11.5308	0.7243	0.7412	–0.0169
45	2,2,6–trimethylheptane	2.1431	–11.5376	0.7200	0.7387	–0.0187
46	2,3,3–trimethylheptane	2.2674	–11.5794	0.7450	0.7417	0.0033
47	2,3,4–trimethylheptane	2.2022	–11.5152	0.7447	0.7432	0.0015

Table 4. (Continued)

No	RH	ΣX_{1CC}	ΣX_{1CH}	$D_{exp.}$ (g/cm^3)	D_{calc} [a] (g/cm^3)	Δ [b]
48	2,3,5–trimethylheptane	2.1672	–11.5210	0.7413	0.7410	0.0003
49	2,3,6–trimethylheptane	2.1216	–11.5287	0.7305	0.7383	–0.0078
50	2,4,4–trimethylheptane	2.2480	–11.5188	0.7308	0.7452	–0.0144
51	2,4,5–trimethylheptane	2.1754	–11.5197	0.7373	0.7415	–0.0042
52	2,4,6–trimethylheptane	2.1189	–11.5273	0.7190	0.7382	–0.0192
53	2,5,5–trimethylheptane	2.2158	–11.5259	0.7362	0.7431	–0.0069
54	3,3,4–trimethylheptane	2.2176	–11.5110	0.7527	0.7442	0.0085
55	3,4,4–trimethylheptane	2.3170	–11.5096	0.7535	0.7493	0.0042
56	3,4,5trimethylheptane	2.2352	–11.5108	0.7519	0.7451	0.0068
57	3–ethyl–2–methyl–heptane	2.0741	–11.5162	0.7398	0.7368	0.0030
58	4–ethyl–2–methyl–heptane	2.0602	–11.5178	0.7322	0.7361	–0.0039
59	5–ethyl–2–methyl–heptane	2.0346	–11.5237	0.7318	0.7344	–0.0026
60	3–ethyl–3–methyl–heptane	2.1826	–11.5132	0.7463	0.7423	0.0040
61	4–ethyl–3–methyl–heptane	2.1204	–11.5095	0.7466	0.7396	0.0070
62	5–ethyl–3–methyl–heptane	2.0804	–11.5952	0.7368	0.7316	0.0052
63	3–ethyl–4–methyl–heptane	2.1159	–11.5106	0.7468	0.7393	0.0075
64	4–ethyl–4–methyl–heptane	2.2037	–11.5087	0.7472	0.7437	0.0035
65	4–propylheptane	1.9584	–11.5144	0.7321	0.7314	0.0007
66	4–isopropylheptane	2.0915	–11.7131	0.7354	0.7239	0.0115
67	2,2,3,3–tetramethylhexane	2.5074	–11.5088	0.7609	0.7589	0.0020
68	2,2,3,4–tetramethylhexane	2.4178	–11.5119	0.7513	0.7542	–0.0029
69	2,2,3,5–tetramethylhexane	2.3552	–11.5217	0.7336	0.7503	–0.0167
70	2,2,4,4–tetramethylhexane	2.4382	–11.5202	0.7424	0.7546	–0.0122
71	2,2,4,5–tetramethylhexane	2.3378	–11.5244	0.7316	0.7492	–0.0176
72	2,2,5,5–tetramethylhexane	2.3523	–11.5340	0.7148	0.7492	–0.0344
73	2,3,3,4–tetramethylhexane	2.4615	–11.5143	0.7656	0.7562	0.0094
74	2,3,3,5–tetramethylhexane	2.3895	–11.5158	0.7449	0.7524	–0.0075
75	2,3,4,4–tetramethylhexane	2.4442	–11.5083	0.7586	0.7558	0.0028
76	2,3,4,5–tetramethylhexane	2.3348	–11.5124	0.7456	0.7499	–0.0043
77	3,3,4,4–tetramethylhexane	2.5621	–11.5018	0.7789	0.7623	0.0166
78	2,2–dimethyl–3–ethyl–hexane	2.2189	–11.5105	0.7447	0.7443	0.0004
79	2,3–dimethyl–3–ethyl–hexane	2.3488	–11.5047	0.7599	0.7512	0.0087
80	2,3–dimethyl–4–ethyl–hexane	2.2483	–11.5085	0.7516	0.7459	0.0057
81	2,4–dimethyl–3 –ethyl–hexane	2.2569	–11.5071	0.7514	0.7464	0.0050
82	2,4–dimethyl–4 –ethyl–hexane	2.3046	–11.5116	0.7525	0.7485	0.0040
83	2,5 –dimethyl– 3 –ethyl–hexane	2.1932	–11.5159	0.7368	0.7427	–0.0059
84	3,3 –dimethyl– 4 –ethyl–hexane	2.3590	–11.5038	0.7598	0.7518	0.0080
85	3,4 –dimethyl– 3 –ethyl–hexane	2.3772	–11.5016	0.7596	0.7529	0.0067
86	3,3–diethylhexane	2.2645	–11.5010	0.7575	0.7473	0.0102
87	3,4–diethylhexane	2.1626	–11.3856	0.7472	0.7507	–0.0035
88	2–methyl–3–isopropyl hexane	2.2279	–11.5102	0.7436	0.7448	–0.0012
89	2,2,3,3,4–pentapentane	2.6542	–11.3029	0.7767	0.7827	–0.0060
90	2,2,3,4,4–pentapentane	2.6037	–11.5120	0.7636	0.7637	–0.0001
91	2,2,3–trimethyl–3–ethyl–pentane	2.5709	–11.4998	0.7780	0.7629	0.0151
92	2,3,4–trimethyl–3–ethyl–pentane	2.4966	–11.4999	0.7735	0.7591	0.0144
93	2–methyl–3,3–diethyl–pentane	2.4130	–11.4958	0.7755	0.7551	0.0204
94	2,4–dimethyl–3–isopropyl–pentane	2.3679	–11.5060	0.7545	0.7521	0.0024

[a] Calculated by Eq. (5). [b] $\Delta = D_{exp.} - D_{calc}$.

Taking some measured densities [8] (at 1 atm and 20 ^oC) of various sorts of monosubsituted alkanes RX as data set (listed in Table 5), using Eq. (7) as the model, we obtained the following correlation expression

$$D_{RX} = \frac{M_{RX}}{1.5466 + 19.5174 r_X + 16.6900 PEI - 5.3779 PEI \times \chi_X - 7.5257 \Sigma X_{1CC} - 17.8716 \Sigma X_{1CH}} \quad (8)$$

$$n = 213 \quad R = 0.996 \quad R^2_A = 0.991 \quad \mathrm{F} = 25568 \quad SEE = 0.0211$$
$$PRESS = 0.0106 \quad SSY = 193.719 \quad R^2_{CV} = 0.9995 \quad S_{PRESS} = 0.0226 \quad PSE = 0.0223$$

For the data set including 213 compounds RX (X= NH2, OH, SH, F, Cl, Br, I) and the density range from 0.6 to 2.3 g/cm^3, the correlation coefficient is good (R = 0.996). Using Eq. (8) to estimate the density for RX (the estimated densities can be seen in Table 5), we get the results of the root–mean–square error (rms), the average absolute error and the average relative error being only 0.0208 g/cm^3, 0.0171 g/cm^3 and 1.85% between the experimental and estimated values respectively. Figure 1 shows the plot of experimental densities versus calculated ones (determined by Eq. (8)) of monosubstituted alkanes. The straight line represents an exact prediction. From Table 5 and Figure 1, one can see that the estimated densities agree with experimental ones well. The stability of Eq. (8) was tested by LOO cross–validation. the statistics of LOO cross–validation shows that Eq. (8) is a stable model for predicting the density of RX.

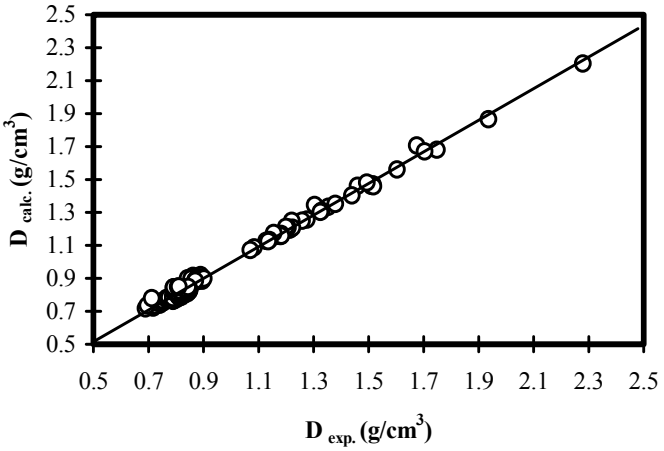

Figure 1. The plot of calculated (by Eq. (8)) vs. experimental densities of monosubstituted alkanes RX.

Karelson *et al*. [2] ever proposed a 4–parameter model to estimate the densities for organic compounds containing S, O, and halogen atoms, and got a good result with the standard error s=0.036 g/cm^3. Compared with Karelson's result, the predictive precision of this work is better.

Not only can Eq. (8) give a satisfying result, but also each item of Eq. (8) has a very explicit physical meaning. In our previous work [5], we have demonstrated that X_{1CC} and X_{1CH} correlate with the energy of C–C and C–H bond of an alkane molecule, respectively. As we know, there is a proportion by inversion between bond energy and bond length for a same sort of bond. That is to say, the lower the bond energy is, the longer the bond length will be for the same sort of bond. Thus, in view of this point, the eigenvalues of orbital–connecting matrices ΣX_{1CC} and ΣX_{1CH} represent the contributions of all C–C and C–H bonds of a compound to the molar volume; r_X scales the contribution of substituent X to the molar volume of the compound RX.

Table 5. Experimental and estimated density (at 1 atm and 20 °C) for 213 monosubstituted alkanes

No	RX	PEI	r_x [a]	ΣX_{1CC}	ΣX_{1CH}	$D_{exp.}$ ($g \cdot cm^{-3}$)	$D_{calc.}$ [b] ($g \cdot cm^{-3}$)	Δ [c]
1	propylamine	1.1887	0.54	0.1356	–3.9385	0.7173	0.7208	–0.0035
2	isopropylamine	1.2810	0.54	0.1356	–3.9604	0.6891	0.7171	–0.0280
3	butylamine	1.2122	0.54	0.3203	–4.9612	0.7414	0.7392	0.0022
4	*sec*–butylanime	1.3292	0.54	0.3203	–4.9881	0.7246	0.7353	–0.0107
5	*tert*–butylamine	1.4215	0.54	0.3921	–5.0166	0.6958	0.7353	–0.0395
6	pentylamine	1.2260	0.54	0.5296	–5.9741	0.7544	0.7546	–0.0002
7	1–methyl–butylamine	1.3527	0.54	0.5296	–6.0031	0.7348	0.7510	–0.0162
8	1–ethyl–propylamine	1.3773	0.54	0.5296	–6.0085	0.7487	0.7503	–0.0016
9	3–methyl–butylamine	1.2357	0.54	0.6219	–5.9831	0.7505	0.7581	–0.0076
10	hexylamine	1.2350	0.54	0.7533	–6.9826	0.7660	0.7673	–0.0013
11	1–methyl–pentylamine	1.3665	0.54	0.7533	–7.0125	0.7533	0.7639	–0.0106
12	3–methyl–pentylamine	1.2495	0.54	0.8753	–6.9896	0.7670	0.7719	–0.0049
13	1,2,2–trimethyl–propylamine	1.4254	0.54	1.0264	–7.0553	0.7688	0.7714	–0.0026
14	heptylamine	1.2414	0.54	0.9866	–7.9861	0.7754	0.7780	–0.0026
15	1–propyl–butylamine	1.4243	0.54	0.9866	–8.0269	0.7670	0.7739	–0.0069
16	4–methyl–hexylamine	1.2488	0.54	1.1214	–7.9889	0.7802	0.7831	–0.0029
17	1,3–dimethyl–pentyamine	1.3900	0.54	1.1214	–8.0206	0.7655	0.7799	–0.0144
18	1,1,3–trimethyl–butylamine	1.5167	0.54	1.1998	–8.0519	0.7119	0.7798	–0.0679
19	octylamine	1.2461	0.54	1.2266	–8.9872	0.7826	0.7871	–0.0045
20	1–methyl–heptylamine	1.3819	0.54	1.2266	–9.0179	0.7744	0.7842	–0.0098
21	1–methyl–octylamine	1.2498	0.54	1.4718	–9.9849	0.7886	0.7950	–0.0064
22	methanol	1.0000	0.46	0.0000	–1.8540	0.7914	0.7647	0.0267
23	ethanol	1.1405	0.46	0.0000	–2.9045	0.7893	0.7620	0.0273
24	propanol	1.1887	0.46	0.1356	–3.9385	0.7997	0.7718	0.0279
25	butanol	1.2122	0.46	0.3203	–4.9612	0.8098	0.7824	0.0274
26	butan–2–ol	1.3292	0.46	0.3203	–4.9881	0.8063	0.7802	0.0261
27	2–methyl–propanol	1.2368	0.46	0.3921	–4.9753	0.8018	0.7851	0.0167
28	2–methyl–propan–2–ol	1.4215	0.46	0.3921	–5.0166	0.7887	0.7818	0.0069
29	pentanol	1.2260	0.46	0.5296	–5.9741	0.8144	0.7922	0.0222
30	pentan–2–ol	1.3527	0.46	0.5296	–6.0031	0.8094	0.7901	0.0193
31	pentan–3–ol	1.3773	0.46	0.5296	–6.0085	0.8203	0.7898	0.0305
32	2,2–dimethyl–propan–1–ol	1.2849	0.46	0.7552	–6.0071	0.8120	0.8009	0.0111
33	3–methyl–butanol	1.2357	0.46	0.6219	–5.9831	0.8104	0.7961	0.0143
34	2–methyl–butan–2–ol	1.4697	0.46	0.6219	–6.0346	0.8096	0.7926	0.0170
35	3–methyl–butan–2–ol	1.3773	0.46	0.6219	–6.0152	0.8180	0.7938	0.0242
36	hexanol	1.2350	0.46	0.7533	–6.9826	0.8136	0.8006	0.0130
37	hexan–2–ol	1.3665	0.46	0.7533	–7.0125	0.8159	0.7987	0.0172
38	2–methyl–pentanol	1.2741	0.46	0.8540	–6.9967	0.8263	0.8042	0.0221
39	3–methyl–pentanol	1.2495	0.46	0.8753	–6.9896	0.8242	0.8057	0.0185
40	4–methyl–pentan–1–ol	1.2398	0.46	0.8540	–6.9886	0.8131	0.8047	0.0084
41	3–methyl–pentan–2–ol	1.4008	0.46	0.8753	–7.0235	0.8307	0.8036	0.0271
42	4–methyl–pentan–2–ol	1.3762	0.46	0.8540	–7.0195	0.8075	0.8028	0.0047
43	2–methyl–pentan–3–ol	1.4254	0.46	0.8540	–7.0300	0.8243	0.8022	0.0221
44	3–methyl–pentan–3–ol	1.5178	0.46	0.8753	–7.0476	0.8286	0.8023	0.0263
45	2,2–dimethyl–butanol	1.3084	0.46	1.0264	–7.0298	0.8283	0.8091	0.0192
46	2,3–dimethyl–butan–1–ol	1.2838	0.46	0.9654	–7.0005	0.8297	0.8092	0.0205
47	2,3–dimethyl–butan–2–ol	1.5178	0.46	0.9654	–7.0532	0.8236	0.8059	0.0177
48	2–ethyl–butan–1–ol	1.2838	0.46	0.8753	–6.9976	0.8326	0.8052	0.0274
49	heptan–1–ol	1.2414	0.46	0.9866	–7.9861	0.8219	0.8079	0.0140
50	heptan–2–ol	1.3755	0.46	0.9866	–8.0165	0.8167	0.8062	0.0105
51	heptan–4–ol	1.4243	0.46	0.9866	–8.0269	0.8183	0.8057	0.0126
52	2–methyl–hexanol	1.2831	0.46	1.0914	–8.0003	0.8270	0.8114	0.0156
53	3–methyl–hexanol	1.2585	0.46	1.1214	–7.9911	0.8258	0.8133	0.0125
54	4–methyl–hexanol	1.2488	0.46	1.1214	–7.9889	0.8239	0.8135	0.0104
55	5–methyl–hexanol	1.2440	0.46	1.0914	–7.9912	0.8119	0.8119	0.0000

Table 5. (Continued)

No	RX	PEI	r_x [a]	ΣX_{1CC}	ΣX_{1CH}	$D_{exp.}$ ($g \cdot cm^{-3}$)	$D_{calc.}$ [b] ($g \cdot cm^{-3}$)	Δ [c]
56	2–methyl–hexan–2–ol	1.5070	0.46	1.0914	–8.0483	0.8119	0.8088	0.0031
57	5–methyl–hexan–2–ol	1.3803	0.46	1.0914	–8.0220	0.8140	0.8102	0.0038
58	2–methyl–hexan–3–ol	1.4489	0.46	1.0914	–8.0365	0.8407	0.8094	0.0313
59	3–methyl–hexan–3–ol	1.5413	0.46	1.1214	–8.0516	0.8233	0.8101	0.0132
60	5–methyl–hexan–3–ol	1.4243	0.46	1.0914	–8.0314	0.8270	0.8097	0.0173
61	2,4–dimethyl–pentanol	1.2879	0.46	1.1998	–8.0032	0.7930	0.8158	–0.0228
62	2,4–dimethyl–pentan–2–ol	1.5167	0.46	1.1998	–8.0519	0.8103	0.8132	–0.0029
63	2,2–dimethyl–pentan–3–ol	1.4735	0.46	1.2794	–8.0462	0.8253	0.8167	0.0086
64	2,4–dimethyl–pentan–3–ol	1.4735	0.46	1.1998	–8.0433	0.8288	0.8136	0.0152
65	octan–2–ol	1.3819	0.46	1.2266	–9.0179	0.8193	0.8127	0.0066
66	octan–3–ol	1.4236	0.46	1.2266	–9.0267	0.8258	0.8123	0.0135
67	octan–4–ol	1.4381	0.46	1.2266	–9.0298	0.8186	0.8122	0.0064
68	6–methyl–heptan–2–ol	1.3845	0.46	1.3335	–9.0214	0.8218	0.8165	0.0053
69	2–methyl–heptan–3–ol	1.4627	0.46	1.3335	–9.0379	0.8235	0.8157	0.0078
70	4–methyl–heptan–4–ol	1.5648	0.46	1.3765	–9.0519	0.8248	0.8171	0.0077
71	2,5–dimethyl–hexanol	1.2921	0.46	1.4418	–9.0037	0.8280	0.8215	0.0065
72	2,3–dimethyl–hexan–2–ol	1.5551	0.46	1.4990	–9.0515	0.8365	0.8218	0.0147
73	2,5–dimethyl–hexan–2–ol	1.5208	0.46	1.4418	–9.0523	0.8227	0.8192	0.0035
74	2,2–dimethyl–hexan–3–ol	1.4970	0.46	1.5296	–9.0474	0.8342	0.8228	0.0114
75	2,5–dimethyl–hexan–3–ol	1.4724	0.46	1.4418	–9.0426	0.8212	0.8196	0.0016
76	3,5–dimethyl–hexan–3–ol	1.5648	0.46	1.4798	–9.0559	0.8373	0.8207	0.0166
77	4,4–dimethyl–hexan–3–ol	1.4970	0.46	1.5865	–9.0399	0.8341	0.8257	0.0084
78	2–ethyl–hexanol	1.3066	0.46	1.3679	–9.0002	0.8319	0.8191	0.0128
79	3–ethyl–hexan–3–ol	1.5894	0.46	1.4112	–9.0524	0.8373	0.8186	0.0187
80	2,4,4–trimethyl–pentan–2–ol	1.5402	0.46	1.6445	–9.0566	0.8225	0.8269	–0.0044
81	2,2,4–trimethyl–pentan–3–ol	1.5216	0.46	1.6445	–9.0530	0.8297	0.8270	0.0027
82	2,3,4–trimethyl–pentan–3–ol	1.6140	0.46	1.6247	–9.0629	0.8492	0.8262	0.0230
83	3–ethyl–2–methyl–pentan–2–ol	1.5648	0.46	1.5374	–9.0484	0.8382	0.8237	0.0145
84	3–ethyl–2–methyl–pentan–3–ol	1.6140	0.46	1.5374	–9.0577	0.8280	0.8233	0.0047
85	nonan–1–ol	1.2498	0.46	1.4718	–9.9849	0.8273	0.8199	0.0074
86	nonan–2–ol	1.3866	0.46	1.4718	–10.0157	0.8471	0.8185	0.0286
87	nonan–3–ol	1.4300	0.46	1.4718	–10.0249	0.8250	0.8181	0.0069
88	nonan–4–ol	1.4471	0.46	1.4718	–10.0285	0.8282	0.8179	0.0103
89	nonan–5–ol	1.4519	0.46	1.4718	–10.0295	0.8356	0.8179	0.0177
90	2–methyl–octan–2–ol	1.5224	0.46	1.5800	–10.0467	0.8210	0.8208	0.0002
91	4–methyl–octan–4–ol	1.5786	0.46	1.6299	–10.0496	0.8267	0.8228	0.0039
92	2,6–dimethyl–heptan–2–ol	1.5250	0.46	1.8132	–10.0486	0.8186	0.8290	–0.0104
93	2,3–dimethyl–heptan–3–ol	1.6032	0.46	1.7312	–10.0541	0.8395	0.8263	0.0132
94	2,6–dimethyl–heptan–3–ol	1.4765	0.46	1.8132	–10.0389	0.8212	0.8294	–0.0082
95	2,4–dimethyl–heptan–4–ol	1.5883	0.46	1.7439	–10.0519	0.8215	0.8268	–0.0053
96	2,6–dimethyl–heptan–4–ol	1.4713	0.46	1.8132	–10.0378	0.8114	0.8295	–0.0181
97	4–ethyl–heptan–4–ol	1.6129	0.46	1.6803	–10.0483	0.8350	0.8250	0.0100
98	2–ethyl–3–methyl–hexan–1–ol	1.3301	0.46	1.7963	–9.9929	0.8486	0.8315	0.0171
99	2,2,3–trimethyl–hexan–3–ol	1.6375	0.46	1.9732	–10.0589	0.8474	0.8349	0.0125
100	2,4,4–trimethyl–hexan–3–ol	1.5451	0.46	1.9640	–10.0422	0.8489	0.8352	0.0137
101	decan–1–ol	1.2527	0.46	1.7204	–10.9812	0.8297	0.8248	0.0049
102	decan–2–ol	1.3903	0.46	1.7204	–11.0121	0.8250	0.8235	0.0015
103	decan–4–ol	1.4535	0.46	1.7204	–11.0254	0.8261	0.8230	0.0031
104	2,7–dimethyl–octan–3–ol	1.4807	0.46	1.9391	–11.0344	0.8152	0.8296	–0.0144
105	2,6–dimethyl–octan–4–ol	1.4851	0.46	1.9780	–11.0300	0.8114	0.8313	–0.0199
106	3–ethyl–2–methyl–heptan–3–ol	1.6513	0.46	2.0741	–11.0451	0.8455	0.8346	0.0109
107	bromomethane	1.0000	1.03	0.0000	–1.8540	1.6755	1.7082	–0.0327
108	bromoethane	1.1405	1.03	0.0000	–2.9045	1.4604	1.4630	–0.0026
109	bromopropane	1.1887	1.03	0.1356	–3.9385	1.3537	1.3368	0.0169
110	2–bromopropane	1.2810	1.03	0.1356	–3.9604	1.3140	1.3301	–0.0161

Table 5. (Continued)

No	RX	PEI	r_x [a]	ΣX_{1CC}	ΣX_{1CH}	$D_{exp.}$ ($g \cdot cm^{-3}$)	$D_{calc.}$ [b] ($g \cdot cm^{-3}$)	Δ [c]
111	bromobutane	1.2122	1.03	0.3203	–4.9612	1.2758	1.2578	0.0180
112	2–bromobutane	1.3292	1.03	0.3203	–4.9881	1.2585	1.2513	0.0072
113	2–bromo–2–methyl–propane	1.4215	1.03	0.3921	–5.0166	1.2209	1.2508	–0.0299
114	bromopentane	1.2260	1.03	0.5296	–5.9741	1.2182	1.2036	0.0146
115	2– bromopentane	1.3527	1.03	0.5296	–6.0031	1.2075	1.1977	0.0098
116	3– bromopentane	1.3773	1.03	0.5296	–6.0085	1.2140	1.1966	0.0174
117	1–bromo–2–methyl–butane	1.2603	1.03	0.6219	–5.9889	1.2234	1.2075	0.0159
118	1–bromo–3–methyl–butane	1.2357	1.03	0.6219	–5.9831	1.2071	1.2087	–0.0016
119	1–bromo–2,2–dimethyl–propane	1.2849	1.03	0.7552	–6.0071	1.1997	1.2139	–0.0142
120	bromohexane	1.2350	1.03	0.7533	–6.9826	1.1744	1.1635	0.0109
121	2– bromohexane	1.3665	1.03	0.7533	–7.0125	1.1658	1.1583	0.0075
122	3– bromohexane	1.4008	1.03	0.7533	–7.0199	1.1799	1.1570	0.0229
123	1–bromo–2–methyl–pentane	1.2741	1.03	0.8540	–6.9967	1.1624	1.1675	–0.0051
124	1–bromo–3–methyl–pentane	1.2495	1.03	0.8753	–6.9896	1.1829	1.1700	0.0129
125	1–bromo–4–methyl–pentane	1.2398	1.03	0.8540	–6.9886	1.1683	1.1689	–0.0006
126	3–bromo–3–methyl–pentane	1.5178	1.03	0.8753	–7.0476	1.1835	1.1598	0.0237
127	1–bromo–3,3–dimethyl–butane	1.2592	1.03	1.0264	–7.0130	1.1556	1.1759	–0.0203
128	1–bromoheptane	1.2414	1.03	0.9866	–7.9861	1.1400	1.1329	0.0071
129	2–bromoheptane	1.3755	1.03	0.9866	–8.0165	1.1277	1.1283	–0.0006
130	4–bromoheptane	1.4243	1.03	0.9866	–8.0269	1.1351	1.1267	0.0084
131	1–bromononane	1.2498	1.03	1.4718	–9.9849	1.0840	1.0890	–0.0050
132	1–bromodecane	1.2527	1.03	1.7204	–10.9812	1.0702	1.0727	–0.0025
133	1–chloropropane	1.1887	0.78	0.1356	–3.9385	0.8899	0.9152	–0.0253
134	2–chloropropane	1.2810	0.78	0.1356	–3.9604	0.8617	0.9113	–0.0496
135	1–chlorobutane	1.2122	0.78	0.3203	–4.9612	0.8862	0.9011	–0.0149
136	2–chlorobutane	1.3292	0.78	0.3203	–4.9881	0.8732	0.8972	–0.0240
137	1–chloro–2–methyl–propane	1.2368	0.78	0.3921	–4.9753	0.8773	0.9037	–0.0264
138	2–chloro–2–methyl–propane	1.4215	0.78	0.3921	–5.0166	0.8420	0.8977	–0.0557
139	1–chloropentane	1.2260	0.78	0.5296	–5.9741	0.8820	0.8936	–0.0116
140	2–chloropentane	1.3527	0.78	0.5296	–6.0031	0.8698	0.8900	–0.0202
141	3–chloropentane	1.3773	0.78	0.5296	–6.0085	0.8731	0.8894	–0.0163
142	1–chloro–3–methyl–butane	1.2357	0.78	0.6219	–5.9831	0.8750	0.8977	–0.0227
143	2–chloro–2–methyl–butane	1.4697	0.78	0.6219	–6.0346	0.8653	0.8913	–0.0260
144	1–chloro–2,2–dimethyl–propane	1.2849	0.78	0.7552	–6.0071	0.8660	0.9021	–0.0361
145	1–chlorohexane	1.2350	0.78	0.7533	–6.9826	0.8785	0.8892	–0.0107
146	3–chlorohexane	1.4008	0.78	0.7533	–7.0199	0.8684	0.8852	–0.0168
147	2–chloro–2–methyl–pentane	1.4932	0.78	0.8540	–7.0439	0.8630	0.8875	–0.0245
148	2–chloro–4–methyl–pentane	1.3762	0.78	0.8540	–7.0195	0.8610	0.8901	–0.0291
149	1–chloro–2–ethyl–butane	1.2838	0.78	0.8753	–6.9976	0.8914	0.8936	–0.0022
150	3–chloro–3–methyl–pentane	1.5178	0.78	0.8753	–7.0476	0.8900	0.8882	0.0018
151	1–chloro–3,3–dimethyl–butane	1.2592	0.78	1.0264	–7.0130	0.8670	0.8993	–0.0323
152	2–chloro–2,3–dimethyl–butane	1.5178	0.78	0.9654	–7.0532	0.8780	0.8920	–0.0140
153	3–chloro–2,2–dimethyl–butane	1.4254	0.78	1.0264	–7.0553	0.8767	0.8946	–0.0179
154	1–chloroheptane	1.2414	0.78	0.9866	–7.9861	0.8758	0.8867	–0.0109
155	2–chloroheptane	1.3755	0.78	0.9866	–8.0165	0.8672	0.8837	–0.0165
156	3–chloroheptane	1.4146	0.78	0.9866	–8.0249	0.8960	0.8829	0.0131
157	4–chloroheptane	1.4243	0.78	0.9866	–8.0269	0.8710	0.8827	–0.0117
158	1–chloro–3–methyl–hexane	1.2585	0.78	1.1214	–7.9911	0.8766	0.8921	–0.0155
159	2–chloro–2–methyl–hexane	1.5070	0.78	1.0914	–8.0483	0.8635	0.8853	–0.0218
160	2–chloro–5–methyl–hexane	1.3803	0.78	1.0914	–8.0220	0.8630	0.8878	–0.0248
161	3–chloro–3–methyl–hexane	1.5413	0.78	1.1214	–8.0516	0.8787	0.8863	–0.0076
162	2–chloro–2,4–dimethyl–pentane	1.5167	0.78	1.1998	–8.0519	0.8610	0.8897	–0.0287
163	4–chloro–2,2–dimethyl–pentane	1.3997	0.78	1.2794	–8.0308	0.8550	0.8952	–0.0402
164	3–chloro–3–ethyl–pentane	1.5659	0.78	1.1517	–8.0529	0.8856	0.8875	–0.0019
165	1–chlorooctane	1.2461	0.78	1.2266	–8.9872	0.8738	0.8851	–0.0113

Table 5. (Continued)

No	RX	PEI	r_x [a]	ΣX_{1CC}	ΣX_{1CH}	$D_{exp.}$ ($g\cdot cm^{-3}$)	$D_{calc.}$ [b] ($g\cdot cm^{-3}$)	Δ [c]
166	3–chloro–3–methyl–heptane	1.5551	0.78	1.3679	–9.0522	0.8764	0.8851	–0.0087
167	4–chloro–4–methyl–heptane	1.5648	0.78	1.3765	–9.0519	0.8690	0.8855	–0.0165
168	3–chloro–2,3–dimethyl–hexane	1.5894	0.78	1.4990	–9.0581	0.8869	0.8898	–0.0029
169	1–chloro–2–ethyl–hexane	1.3066	0.78	1.3679	–9.0002	0.8769	0.8896	–0.0127
170	2–chloro–2,4,4–trimethyl–pentane	1.5402	0.78	1.6445	–9.0566	0.8746	0.8958	–0.0212
171	1–chlorononane	1.2498	0.78	1.4718	–9.9849	0.8720	0.8843	–0.0123
172	2–chlorononane	1.3866	0.78	1.4718	–10.0157	0.8790	0.8819	–0.0029
173	4–chloro–4–methyl–octane	1.5786	0.78	1.6299	–10.0496	0.8723	0.8849	–0.0126
174	3–chloro–3–ethyl–heptane	1.6032	0.78	1.6668	–10.0496	0.8856	0.8863	–0.0007
175	3–chloro–2,2,3–dimethyl–hexane	1.6375	0.78	1.9732	–10.0589	0.9010	0.8968	0.0042
176	1–chlorodecane	1.2527	0.78	1.7204	–10.9812	0.8705	0.8839	–0.0134
177	iodomethane	1.0000	1.39	0.0000	–1.8540	2.2790	2.2105	0.0685
178	iodoethane	1.1405	1.39	0.0000	–2.9045	1.9358	1.8715	0.0643
179	1–iodopropane	1.1887	1.39	0.1356	–3.9385	1.7489	1.6842	0.0647
180	2–iodopropane	1.2810	1.39	0.1356	–3.9604	1.7042	1.6741	0.0301
181	1–iodo–2–methyl–propane	1.2368	1.39	0.3921	–4.9753	1.6035	1.5639	0.0396
182	1–iodopentane	1.2260	1.39	0.5296	–5.9741	1.5161	1.4727	0.0434
183	2–iodopentane	1.3527	1.39	0.5296	–6.0031	1.5096	1.4637	0.0459
184	3–iodopentane	1.3773	1.39	0.5296	–6.0085	1.5176	1.4621	0.0555
185	1–iodo–2,2–dimethyl–propane	1.2849	1.39	0.7552	–6.0071	1.4940	1.4834	0.0106
186	1–iodohexane	1.2350	1.39	0.7533	–6.9826	1.4397	1.4057	0.0340
187	1–iodoheptane	1.2414	1.39	0.9866	–7.9861	1.3791	1.3532	0.0259
188	2–iodoheptane	1.3755	1.39	0.9866	–8.0165	1.3040	1.3463	–0.0423
189	1–iodooctane	1.2461	1.39	1.2266	–8.9872	1.3297	1.3107	0.0190
190	2–iodooctane	1.3819	1.39	1.2266	–9.0179	1.3251	1.3045	0.0206
191	propanethiol	1.1887	0.87	0.1356	–3.9385	0.8411	0.8330	0.0081
192	propane–2–thiol	1.2810	0.87	0.1356	–3.9604	0.8143	0.8271	–0.0128
193	butane–1–thiol	1.2122	0.87	0.3203	–4.9612	0.8416	0.8318	0.0098
194	butane–2–thiol	1.3292	0.87	0.3203	–4.9881	0.8295	0.8257	0.0038
195	2–methyl–propanethiol	1.2368	0.87	0.3921	–4.9753	0.8357	0.8335	0.0022
196	2–methyl–propane–2–thiol	1.4215	0.87	0.3921	–5.0166	0.7943	0.8239	–0.0296
197	pentane–1–thiol	1.2260	0.87	0.5296	–5.9741	0.8500	0.8336	0.0164
198	pentane–2–thiol	1.3527	0.87	0.5296	–6.0031	0.8327	0.8278	0.0049
199	pentane–3–thiol	1.3773	0.87	0.5296	–6.0085	0.8410	0.8267	0.0143
200	2–methyl–butane–1–thiol	1.2603	0.87	0.6219	–5.9889	0.8420	0.8358	0.0062
201	3–methyl–butane–1–thiol	1.2357	0.87	0.6219	–5.9831	0.8350	0.8370	–0.0020
202	2–methyl–butane–2–thiol	1.4697	0.87	0.6219	–6.0346	0.8120	0.8265	–0.0145
203	hexane–1–thiol	1.2350	0.87	0.7533	–6.9826	0.8424	0.8361	0.0063
204	hexane–2–thiol	1.3665	0.87	0.7533	–7.0125	0.8345	0.8308	0.0037
205	heptane–1–thiol	1.2414	0.87	0.9866	–7.9861	0.8427	0.8390	0.0037
206	octane–1–thiol	1.2461	0.87	1.2266	–8.9872	0.8433	0.8419	0.0014
207	octane–2–thiol	1.3819	0.87	1.2266	–9.0179	0.8366	0.8374	–0.0008
208	decane–1–thiol	1.2527	0.87	1.7204	–10.9812	0.8443	0.8473	–0.0030
209	1–fluropentane	1.2260	0.41	0.5296	–5.9741	0.7907	0.8447	–0.0540
210	1–flurohexane	1.2350	0.41	0.7533	–6.9826	0.7995	0.8466	–0.0471
211	2–flurohexane	1.3665	0.41	0.7533	–7.0125	0.7916	0.8472	–0.0556
212	1–fluroheptane	1.2414	0.41	0.9866	–7.9861	0.8062	0.8489	–0.0427
213	1–flurooctane	1.2461	0.41	1.2266	–8.9872	0.8108	0.8513	–0.0405

[a] from ref. [9]. [b] Calculated by Eq. (8). [c] $\Delta = D_{exp.} - D_{calc.}$

The larger r_X, and the longer C–X bond, will result in a larger contribution to the molar volume. For the two items PEI×χ_x and PEI, its physical meaning can be explained as following: distribution of the electronic cloud of C–C and C–H will be changed and result in the stretch of C–C and C–H

bonds when a hydrogen atom of the nonpolar alkane is replaced with a polar substituent X, which will result in the volume change of the alkyl R eventually. That is to say, PEI×χ_x together with PEI contributes the perturbation volume ΔΔV from RH to RX system, which is caused by the H atom changing into the substituent X.

Table 6. The predicted density (25°C) with Eq. (5) for 160 alkanes. The first five alkanes are in gas phase at 25°C.

No	Alkane	D_{pred} (g cm^{-3})
1	methane	–
2	ethane	–
3	propane	–
4	butane	–
5	2–methylpropane	–
6	pentane	0.6030
7	2–methylbutane	0.6082
8	2,2–dimehtylpropane	0.6156
9	hexane	0.6357
10	2–methylpentane	0.6412
11	3–methylpentane	0.6426
12	2,2–dimehtylbutane	0.6493
13	2,3–dimethylbutane	0.6475
14	heptane	0.6625
15	2–methylhexane	0.6678
16	3–methylhexane	0.6698
17	2,2–dimethylpentane	0.6780
18	2,3–dimethylpentane	0.6763
19	2,4–dimethylpentane	0.6737
20	3,3–dimethylpentane	0.6806
21	3–ethylpentane	0.6717
22	2,2,3–trimethylbutane	0.6852
23	octane	0.6846
24	2–methylheptane	0.6899
25	3–methylheptane	0.6920
26	4–methylheptane	0.6926
27	2,2–dimethylhexane	0.7000
28	2,3–dimethylhexane	0.6989
29	2,4–dimethylhexane	0.6977
30	2,5–dimethylhexane	0.6953
31	3,3–dimethylhexane	0.7036
32	3,4–dimethylhexane	0.7008
33	3–ethylhexane	0.6947
34	2,2,3–trimethylpentane	0.7087
35	2,2,4–trimethylpentane	0.7061
36	2,3,3–trimethylpentane	0.7110
37	2,3,4–trimethylpentane	0.7056
38	3–ethyl–2–methylpentane	0.7013
39	3–ethyl–3–methylpentane	0.7066
40	2,2,3,3–tetramethylbutane	0.7196
41	nonane	0.7035
42	2–methyloctane	0.7085
43	3–methyloctane	0.7107
44	4–methyloctane	0.7109
45	2,2–dimethylheptane	0.7183
46	2,3–dimethylheptane	0.7165
47	2,4–dimethylheptane	0.7171
48	2,5–dimethylheptane	0.7214

Table 6. (Continued)

No	Alkane	D_{pred} (g cm^{-3})
49	2,6–dimethylheptane	0.7199
50	3,3–dimethylheptane	0.7223
51	3,4–dimethylheptane	0.7202
52	3,5–dimethylheptane	0.7185
53	4,4–dimethylheptane	0.7234
54	3–ethylheptane	0.7137
55	4–ethylheptane	0.7146
56	2,2,3–trimethylhexane	0.7289
57	2,2,4–trimethylhexane	0.7267
58	2,2,5–trimethylhexane	0.7239
59	2,3,3–trimethylhexane	0.7306
60	2,3,4–trimethylhexane	0.7268
61	2,3,5–trimethylhexane	0.7234
62	2,4,4–trimethylhexane	0.7283
63	3,3,4–trimethylhexane	0.7323
64	3–ethyl–2–methylhexane	0.7210
65	4–ethyl–2–methylhexane	0.7186
66	3–ethyl–3–methylhexane	0.7266
67	4–ethyl–2–methylhexane	0.7228
68	2,2,3,3–tetramethylpentane	0.7421
69	2,2,3,4–tetramethylpentane	0.7334
70	2,2,4,4–tetramethylpentane	0.7353
71	2,3,3,4–tetramethylpentane	0.7382
72	2,2–dimethyl–3–ethylpentane	0.7318
73	2,3–dimethyl–3–ethylpentane	0.7331
74	2,4–dimethyl–3–ethylpentane	0.7265
75	3,3–diethylpentane	0.7300
76	decane	0.7197
77	2–methylnonane	0.7245
78	3–methylnonane	0.7266
79	4–methylnonane	0.7276
80	5–methylnonane	0.7279
81	2,2–dimethyloctane	0.7339
82	2,3–dimethyloctane	0.7334
83	2,4–dimethyloctane	0.7325
84	2,5–dimethyloctane	0.7328
85	2,6–dimethyloctane	0.7316
86	2,7–dimethyloctane	0.7295
87	3,3–dimethyloctane	0.7379
88	3,4–dimethyloctane	0.7363
89	3,5–dimethyloctane	0.7353
90	3,6–dimethyloctane	0.7340
91	4,4–dimethyloctane	0.7396
92	4,5–dimethyloctane	0.7371
93	3–ethyloctane	0.7297
94	4–ethyloctane	0.7310
95	2,2,3–trimethylheptane	0.7435
96	2,2,4–trimethylheptane	0.7431
97	2,2,5–trimethylheptane	0.7416
98	2,2,6–trimethylheptane	0.7391
99	2,3,3–trimethylheptane	0.7420
100	2,3,4–trimethylheptane	0.7435
101	2,3,5–trimethylheptane	0.7414
102	2,3,6–trimethylheptane	0.7387
103	2,4,4–trimethylheptane	0.7455
104	2,4,5–trimethylheptane	0.7419

Table 6. (Continued)

No	Alkane	D_{pred} (g cm^{-3})
105	2,4,6–trimethylheptane	0.7387
106	2,5,5–trimethylheptane	0.7434
107	3,3,4–trimethylheptane	0.7446
108	3,3,5–trimethylheptane	0.7463
109	3,4,4–trimethylheptane	0.7495
110	3,4,5–trimethylheptane	0.7454
111	3–ethyl–2–methylheptane	0.7373
112	4–ethyl–2–methylheptane	0.7366
113	5–ethyl–2–methylheptane	0.7349
114	3–ethyl–3–methylheptane	0.7427
115	4–ethyl–3–methylheptane	0.7400
116	5–ethyl–3–methylheptane	0.7321
117	3–ethyl–4–methylheptane	0.7397
118	4–ethyl–4–methylheptane	0.7441
119	4–propylheptane	0.7320
120	4–isopropylheptane	0.7244
121	2,2,3,3–tetramethylhexane	0.7590
122	2,2,3,4–tetramethylhexane	0.7543
123	2,2,3,5–tetramethylhexane	0.7505
124	2,2,4,4–tetramethylhexane	0.7547
125	2,2,4,5–tetramethylhexane	0.7494
126	2,2,5,5–tetramethylhexane	0.7494
127	2,3,3,4–tetramethylhexane	0.7563
128	2,3,3,5–tetramethylhexane	0.7526
129	2,3,4,4–tetramethylhexane	0.7559
130	2,3,4,5–tetramethylhexane	0.7502
131	3,3,4,4–tetramethylhexane	0.7623
132	2,2–dimethyl–3–ethylhexane	0.7447
133	2,2–dimethyl–4–ethylhexane	0.7482
134	2,3–dimethyl–3–ethylhexane	0.7514
135	2,3–dimethyl–4–ethylhexane	0.7462
136	2,4–dimethyl–3–ethylhexane	0.7467
137	2,4–dimethyl–4–ethylhexane	0.7487
138	2,5–dimethyl–3–ethylhexane	0.7430
139	3,3–dimethyl–4–ethylhexane	0.7520
140	3,4–dimethyl–3–ethylhexane	0.7530
141	3,3–diethylhexane	0.7476
142	3,4–diethylhexane	0.7510
143	3–isopropyl–2–methylhexane	0.7451
144	2,2,3,3,4–pentamethylpentane	0.7825
145	2,2,3,4,4–pentamethylpentane	0.7636
146	3–ethyl–2,2,3–trimethylpentane	0.7629
147	3–ethyl–2,2,4–trimethylpentane	0.7559
148	3–ethyl–2,3,4–trimethylpentane	0.7591
149	3,3–diethyl–2–methylpentane	0.7553
150	2,4–dimethyl–3–isopropylpentane	0.7523
151	undecane	0.7337
152	dodecane	0.7461
153	tridecane	0.7570
154	tetradecane	0.7668
155	pentadecane	0.7756
156	hexadecane	0.7835
157	heptadecane	0.7908
158	octadecane	0.7973
159	nonadecane	0.8034
160	eicosane	0.8090

Table 7. Eq. (8) predicted densities (20°C) for monosubstituted alkanes. "–" indicates compounds in gas phase at 20°C.

No	RX	D_{pred} (g cm^{-3})
1	methanol	0.7660
2	ethanol	0.7618
3	propanol	0.7713
4	propan–2–ol	0.7170
5	butanol	0.7818
6	butan–2–ol	0.7792
7	2–methyl–propanol	0.7846
8	2–methyl–propan–2–ol	0.7806
9	pentanol	0.7917
10	pentan–2–ol	0.7893
11	pentan–3–ol	0.7888
12	2,2–dimethyl–propan–1–ol	0.8005
13	3–methyl–butanol	0.7957
14	2–methyl–butan–2–ol	0.7914
15	3–methyl–butan–2–ol	0.7930
16	hexanol	0.8001
17	hexan–2–ol	0.7979
18	2–methyl–pentanol	0.8038
19	3–methyl–pentanol	0.8054
20	4–methyl–pentan–1–ol	0.8044
21	3–methyl–pentan–2–ol	0.8029
22	4–methyl–pentan–2–ol	0.8021
23	2–methyl–pentan–3–ol	0.8013
24	3–methyl–pentan–3–ol	0.8012
25	2,2–dimethyl–butanol	0.8087
26	2,3–dimethyl–butan–1–ol	0.8089
27	2,3–dimethyl–butan–2–ol	0.8049
28	2–ethyl–butan–1–ol	0.8048
29	heptan–1–ol	0.8076
30	heptan–2–ol	0.8056
31	heptan–4–ol	0.8049
32	2–methyl–hexanol	0.8110
33	3–methyl–hexanol	0.8131
34	4–methyl–hexanol	0.8132
35	5–methyl–hexanol	0.8116
36	2–methyl–hexan–2–ol	0.8079
37	5–methyl–hexan–2–ol	0.8096
38	2–methyl–hexan–3–ol	0.8086
39	3–methyl–hexan–3–ol	0.8091
40	5–methyl–hexan–3–ol	0.8090
41	2,4–dimethyl–pentanol	0.8155
42	2,4–dimethyl–pentan–2–ol	0.8123
43	2,2–dimethyl–pentan–3–ol	0.8161
44	2,4–dimethyl–pentan–3–ol	0.8129
45	octan–2–ol	0.8121
46	octan–3–ol	0.8116
47	octan–4–ol	0.8114
48	6–methyl–heptan–2–ol	0.8160
49	2–methyl–heptan–3–ol	0.8151
50	4–methyl–heptan–4–ol	0.8162
51	2,5–dimethyl–hexanol	0.8213
52	2,3–dimethyl–hexan–2–ol	0.8210
53	2,5–dimethyl–hexan–2–ol	0.8184
54	2,2–dimethyl–hexan–3–ol	0.8222
55	2,5–dimethyl–hexan–3–ol	0.8190
56	3,5–dimethyl–hexan–3–ol	0.8199

Table 7. (Continued)

No	RX	D_{pred} (g cm^{-3})
57	4,4–dimethyl–hexan–3–ol	0.8252
58	2–ethyl–hexanol	0.8188
59	3–ethyl–hexan–3–ol	0.8177
60	2,4,4–trimethyl–pentan–2–ol	0.8263
61	2,2,4–trimethyl–pentan–3–ol	0.8265
62	2,3,4–trimethyl–pentan–3–ol	0.8254
63	3–ethyl–2–methyl–pentan–2–ol	0.8229
64	3–ethyl–2–methyl–pentan–3–ol	0.8224
65	nonan–1–ol	0.8196
66	nonan–2–ol	0.8180
67	nonan–3–ol	0.8175
68	nonan–4–ol	0.8173
69	nonan–5–ol	0.8172
70	2–methyl–octan–2–ol	0.8201
71	4–methyl–octan–4–ol	0.8220
72	2,6–dimethyl–heptan–2–ol	0.8284
73	2,3–dimethyl–heptan–3–ol	0.8255
74	2,6–dimethyl–heptan–3–ol	0.8290
75	2,4–dimethyl–heptan–4–ol	0.8261
76	2,6–dimethyl–heptan–4–ol	0.8290
77	4–ethyl–heptan–4–ol	0.8242
78	2–ethyl–3–methyl–hexan–1–ol	0.8313
79	2,2,3–trimethyl–hexan–3–ol	0.8342
80	2,4,4–trimethyl–hexan–3–ol	0.8347
81	decan–1–ol	0.8246
82	decan–2–ol	0.8230
83	decan–4–ol	0.8224
84	2,7–dimethyl–octan–3–ol	0.8291
85	2,6–dimethyl–octan–4–ol	0.8308
86	3–ethyl–2–methyl–heptan–3–ol	0.8339
87	fluromethane	–
88	fluroethane	–
89	1–fluro–propane	–
90	2–fluro–propane	0.7499
91	1–fluro–butane	0.8428
92	2–fluro–butane	0.8429
93	1–fluro–2–methyl–propane	0.8466
94	2–fluro–2–methyl–propane	0.8470
95	1–fluro–pentane	0.8439
96	2–fluro–pentane	0.8441
97	3–fluro–pentane	0.8441
98	1–fluro–2,2–dimethyl–propane	0.8551
99	1–fluro–3–methyl–butane	0.8486
100	2–fluro–2–methyl–butane	0.8492
101	2–fluro–3–methyl–butane	0.8488
102	1–fluro–hexane	0.8459
103	2–fluro–hexane	0.8461
104	1–fluro–2–methyl–pentane	0.8507
105	1–fluro–3–methyl–pentane	0.8520
106	1–fluro–4–methyl–pentane	0.8507
107	2–fluro–3–methyl–pentane	0.8522
108	2–fluro–4–methyl–pentane	0.8509
109	3–fluro–2–methyl–pentane	0.8510
110	3–fluro–3–methyl–pentane	0.8527
111	1–fluro–2,2–dimethyl–butane	0.8568
112	1–fluro–2,3–dimethyl–butane	0.8565

Table 7. (Continued)

No	RX	D_{pred} (g cm^{-3})
113	2–fluro–2,3–dimethyl–butane	0.8568
114	1–fluro–2–ethyl–butane	0.8520
115	1–fluro–heptane	0.8484
116	2–fluro–heptane	0.8485
117	4–fluro–heptane	0.8487
118	1–fluro–2–methyl–hexane	0.8528
119	1–fluro–3–methyl–hexane	0.8546
120	1–fluro–4–methyl–hexane	0.8546
121	1–fluro–5–methyl–hexane	0.8528
122	2–fluro–2–methyl–hexane	0.8534
123	2–fluro–5–methyl–hexane	0.8530
124	3–fluro–2–methyl–hexane	0.8532
125	3–fluro–3–methyl–hexane	0.8554
126	3–fluro–5–methyl–hexane	0.8531
127	1–fluro–2,4–dimethyl–pentane	0.8578
128	2–fluro–2,4–dimethyl–pentane	0.8584
129	3–fluro–2,2–dimethyl–pentane	0.8618
130	3–fluro–2,4–dimethyl–pentane	0.8583
131	2–fluro–octane	0.8509
132	3–fluro–octane	0.8511
133	4–fluro–octane	0.8511
134	2–fluro–6–methyl–heptane	0.8552
135	3–fluro–2–methyl–heptane	0.8554
136	4–fluro–4–methyl–heptane	0.8583
137	1–fluro–2,5–dimethyl–hexane	0.8594
138	2–fluro–2,3–dimethyl–hexane	0.8634
139	2–fluro–2,5–dimethyl–hexane	0.8600
140	3–fluro–2,2–dimethyl–hexane	0.8637
141	3–fluro–2,5–dimethyl–hexane	0.8598
142	3–fluro–3,5–dimethyl–hexane	0.8623
143	3–fluro–4,4–dimethyl–hexane	0.8669
144	1–fluro–2–ethyl–hexane	0.8569
145	3–fluro–3–ethyl–hexane	0.8603
146	2–fluro–2,4,4–trimethyl–pentane	0.8688
147	3–fluro–2,2,4–trimethyl–pentane	0.8687
148	3–fluro–2,3,4–trimethyl–pentane	0.8691
149	2–fluro–3–ethyl–2–methyl–pentane	0.8656
150	3–fluro–3–ethyl–2–methyl–pentane	0.8658
151	1–fluro–nonane	0.8532
152	2–fluro–nonane	0.8534
153	3–fluro–nonane	0.8535
154	4–fluro–nonane	0.8535
155	5–fluro–nonane	0.8536
156	2–fluro–2–methyl–octane	0.8577
157	4–fluro–4–methyl–octane	0.8606
158	2–fluro–2,6–dimethyl–heptane	0.8667
159	3–fluro–2,3–dimethyl–heptane	0.8647
160	3–fluro–2,6–dimethyl–heptane	0.8665
161	4–fluro–2,4–dimethyl–heptane	0.8650
162	4–fluro–2,6–dimethyl–heptane	0.8665
163	4–fluro–4–ethyl–heptane	0.8634
164	1–fluro–2–ethyl–3–methyl–hexane	0.8669
165	3–fluro–2,2,3–trimethyl–hexane	0.8746
166	3–fluro–2,4,4–trimethyl–hexane	0.8737
167	1–fluro–decane	0.8555
168	2–fluro–decane	0.8556

Table 7. (Continued)

No	RX	D_{pred} (g cm^{-3})
169	4–fluro–decane	0.8558
170	3–fluro–2,7–dimethyl–octane	0.8633
171	4–fluro–2,6–dimethyl–octane	0.8652
172	3–fluro–3–ethyl–2–methyl–heptane	0.8707
173	iodomethane	2.2042
174	iodoethane	1.8661
175	1–iodopropane	1.6800
176	2–iodopropane	1.6611
177	1–iodobutane	1.5575
178	2–iodobutane	1.5472
179	1–iodo–2–methyl–propane	1.5606
180	2–iodo–2–methyl–propane	1.5446
181	1–iodopentane	1.4699
182	2–iodopentane	1.4607
183	3–iodopentane	1.4590
184	1–iodo–2,2–dimethyl–propane	1.4808
185	1–iodo–3–methyl–butane	1.4756
186	2–iodo–2–methyl–butane	1.4590
187	2–iodo–3–methyl–butane	1.4654
188	1–iodohexane	1.4034
189	2–iodohexane	1.3953
190	1–iodo–2–methyl–pentane	1.4073
191	1–iodo–3–methyl–pentane	1.4106
192	1–iodo–4–methyl–pentane	1.4095
193	2–iodo–3–methyl–pentane	1.4013
194	2–iodo–4–methyl–pentane	1.4011
195	3–iodo–2–methyl–pentane	1.3981
196	3–iodo–3–methyl–pentane	1.3945
197	1–iodo–2,2–dimethyl–butane	1.4133
198	1–iodo–2,3–dimethyl–butane	1.4145
199	2–iodo–2,3–dimethyl–butane	1.4000
200	1–iodo–2–ethyl–butane	1.4085
201	1–iodoheptane	1.3512
202	methanthiol	0.8824
203	ethanthiol	0.8421
204	propanthiol	0.8330
205	propan–2–thiol	0.8269
206	butanthiol	0.8318
207	butan–2–thiol	0.8255
208	2–methyl–propanthiol	0.8335
209	2–methyl–propan–2–thiol	0.8237
210	pentanthiol	0.8336
211	pentan–2–thiol	0.8276
212	pentan–3–thiol	0.8265
213	2,2–dimethyl–propan–1–thiol	0.8401
214	3–methyl–butanthiol	0.8370
215	2–methyl–butan–2–thiol	0.8262
216	3–methyl–butan–2–thiol	0.8304
217	hexanthiol	0.8361
218	hexan–2–thiol	0.8306
219	2–methyl–pentanthiol	0.8385
220	3–methyl–pentanthiol	0.8407
221	4–methyl–pentan–1–thiol	0.8400
222	3–methyl–pentan–2–thiol	0.8344
223	4–methyl–pentan–2–thiol	0.8343
224	2–methyl–pentan–3–thiol	0.8323

Table 7. (Continued)

No	RX	D_{pred} (g cm^{-3})
225	3–methyl–pentan–3–thiol	0.8298
226	2,2–dimethyl–butanthiol	0.8423
227	2,3–dimethyl–butan–1–thiol	0.8431
228	2,3–dimethyl–butan–2–thiol	0.8333
229	2–ethyl–butan–1–thiol	0.8392
230	heptan–1–thiol	0.8390
231	heptan–2–thiol	0.8340
232	heptan–4–thiol	0.8323
233	2–methyl–hexanthiol	0.8413
234	3–methyl–hexanthiol	0.8438
235	4–methyl–hexanthiol	0.8442
236	5–methyl–hexanthiol	0.8428
237	2–methyl–hexan–2–thiol	0.8332
238	5–methyl–hexan–2–thiol	0.8377
239	2–methyl–hexan–3–thiol	0.8352
240	3–methyl–hexan–3–thiol	0.8336
241	5–methyl–hexan–3–thiol	0.8361
242	2,4–dimethyl–pentanthiol	0.8455
243	2,4–dimethyl–pentan–2–thiol	0.8371
244	2,2–dimethyl–pentan–3–thiol	0.8416
245	2,4–dimethyl–pentan–3–thiol	0.8386
246	octan–2–thiol	0.8373
247	octan–3–thiol	0.8359
248	octan–4–thiol	0.8355
249	6–methyl–heptan–2–thiol	0.8409
250	2–methyl–heptan–3–thiol	0.8384
251	4–methyl–heptan–4–thiol	0.8373
252	2,5–dimethyl–hexanthiol	0.8479
253	2,3–dimethyl–hexan–2–thiol	0.8420
254	2,5–dimethyl–hexan–2–thiol	0.8403
255	2,2–dimethyl–hexan–3–thiol	0.8443
256	2,5–dimethyl–hexan–3–thiol	0.8418
257	3,5–dimethyl–hexan–3–thiol	0.8408
258	4,4–dimethyl–hexan–3–thiol	0.8471
259	2–ethyl–hexanthiol	0.8452
260	3–ethyl–hexan–3–thiol	0.8382
261	2,4,4–trimethyl–pentan–2–thiol	0.8472
262	2,2,4–trimethyl–pentan–3–thiol	0.8478
263	2,3,4–trimethyl–pentan–3–thiol	0.8448
264	3–ethyl–2–methyl–pentan–2–thiol	0.8436
265	3–ethyl–2–methyl–pentan–3–thiol	0.8420
266	nonan–1–thiol	0.8448
267	nonan–2–thiol	0.8405
268	nonan–3–thiol	0.8392
269	nonan–4–thiol	0.8387
270	nonan–5–thiol	0.8385
271	2–methyl–octan–2–thiol	0.8399
272	4–methyl–octan–4–thiol	0.8406
273	2,6–dimethyl–heptan–2–thiol	0.8477
274	2,3–dimethyl–heptan–3–thiol	0.8434
275	2,6–dimethyl–heptan–3–thiol	0.8491
276	2,4–dimethyl–heptan–4–thiol	0.8442
277	2,6–dimethyl–heptan–4–thiol	0.8493
278	4–ethyl–heptan–4–thiol	0.8420
279	2–ethyl–3–methyl–hexan–1–thiol	0.8543
280	2,2,3–trimethyl–hexan–3–thiol	0.8509

Table 7. (Continued)

No	RX	D_{pred} (g cm^{-3})
281	2,4,4–trimethyl–hexan–3–thiol	0.8532
282	decan–1–thiol	0.8474
283	decan–2–thiol	0.8434
284	decan–4–thiol	0.8417
285	2,7–dimethyl–octan–3–thiol	0.8476
286	2,6–dimethyl–octan–4–thiol	0.8491
287	3–ethyl–2–methyl–heptan–3–thiol	0.8490
288	chloromethane	–
289	chloroethane	–
290	1–chloropropane	–
291	2–chloropropane	0.8768
292	1–chlorobutane	0.9046
293	2–chlorobutane	0.9004
294	1–chloro–2–methyl–propane	0.9073
295	2–chloro–2–methyl–propane	0.9007
296	1–chloropentane	0.8967
297	2–chloropentane	0.8928
298	3–chloropentane	0.8920
299	1–chloro–2,2–dimethyl–propane	0.9053
300	1–chloro–3–methyl–butane	0.9008
301	2–chloro–2–methyl–butane	0.8938
302	2–chloro–3–methyl–butane	0.8964
303	1–chlorohexane	0.8919
304	2–chlorohexane	0.8884
305	1–chloro–2–methyl–pentane	0.8953
306	1–chloro–3–methyl–pentane	0.8973
307	1–chloro–4–methyl–pentane	0.8963
308	2–chloro–3–methyl–pentane	0.8932
309	2–chloro–4–methyl–pentane	0.8926
310	3–chloro–2–methyl–pentane	0.8914
311	3–chloro–3–methyl–pentane	0.8903
312	1–chloro–2,2–dimethyl–butane	0.9002
313	1–chloro–2,3–dimethyl–butane	0.9006
314	2–chloro–2,3–dimethyl–butane	0.8942
315	1–chloro–2–ethyl–butane	0.8963
316	1–chloroheptane	0.8891
317	2–chloroheptane	0.8859
318	4–chloroheptane	0.8848
319	1–chloro–2–methyl–hexane	0.8923
320	1–chloro–3–methyl–hexane	0.8947
321	1–chloro–4–methyl–hexane	0.8949
322	1–chloro–5–methyl–hexane	0.8933
323	2–chloro–2–methyl–hexane	0.8872
324	2–chloro–5–methyl–hexane	0.8900
325	3–chloro–2–methyl–hexane	0.8885
326	3–chloro–3–methyl–hexane	0.8882
327	3–chloro–5–methyl–hexane	0.8890
328	1–chloro–2,4–dimethyl–pentane	0.8970
329	2–chloro–2,4–dimethyl–pentane	0.8917
330	3–chloro–2,2–dimethyl–pentane	0.8960
331	3–chloro–2,4–dimethyl–pentane	0.8927
332	2–chlorooctane	0.8844
333	3–chlorooctane	0.8836
334	4–chlorooctane	0.8833
335	2–chloro–6–methyl–heptane	0.8884
336	3–chloro–2–methyl–heptane	0.8868

Table 7. (Continued)

No	RX	D_{pred} (g cm^{-3})
337	4–chloro–4–methyl–heptane	0.8872
338	1–chloro–2,5–dimethyl–hexane	0.8946
339	2–chloro–2,3–dimethyl–hexane	0.8923
340	2–chloro–2,5–dimethyl–hexane	0.8899
341	3–chloro–2,2–dimethyl–hexane	0.8939
342	3–chloro–2,5–dimethyl–hexane	0.8908
343	3–chloro–3,5–dimethyl–hexane	0.8911
344	3–chloro–4,4–dimethyl–hexane	0.8970
345	1–chloro–2–ethyl–hexane	0.8919
346	3–chloro–3–ethyl–hexane	0.8886
347	2–chloro–2,4,4–trimethyl–pentane	0.8978
348	3–chloro–2,2,4–trimethyl–pentane	0.8982
349	3–chloro–2,3,4–trimethyl–pentane	0.8964
350	2–chloro–3–ethyl–2–methyl–pentane	0.8942
351	3–chloro–3–ethyl–2–methyl–pentane	0.8933
352	1–chlorononane	0.8864
353	2–chlorononane	0.8837
354	3–chlorononane	0.8829
355	4–chlorononane	0.8826
356	5–chlorononane	0.8825
357	2–chloro–2–methyl–octane	0.8850
358	4–chloro–4–methyl–octane	0.8866
359	2–chloro–2,6–dimethyl–heptane	0.8935
360	3–chloro–2,3–dimethyl–heptane	0.8900
361	3–chloro–2,6–dimethyl–heptane	0.8944
362	4–chloro–2,4–dimethyl–heptane	0.8906
363	4–chloro–2,6–dimethyl–heptane	0.8945
364	4–chloro–4–ethyl–heptane	0.8886
365	1–chloro–2–ethyl–3–methyl–hexane	0.8978
366	3–chloro–2,2,3–trimethyl–hexane	0.8987
367	3–chloro–2,4,4–trimethyl–hexane	0.8998
368	1–chlorodecane	0.8858
369	2–chlorodecane	0.8833
370	4–chlorodecane	0.8823
371	3–chloro–2,7–dimethyl–octane	0.8890
372	4–chloro–2,6–dimethyl–octane	0.8907
373	3–chloro–3–ethyl–2–methyl–heptane	0.8928
374	2–iodoheptane	1.3441
375	4–iodoheptane	1.3416
376	1–iodo–2–methyl–hexane	1.3548
377	1–iodo–3–methyl–hexane	1.3586
378	1–iodo–4–methyl–hexane	1.3591
379	1–iodo–5–methyl–hexane	1.3570
380	2–iodo–2–methyl–hexane	1.3433
381	2–iodo–5–methyl–hexane	1.3497
382	3–iodo–2–methyl–hexane	1.3461
383	3–iodo–3–methyl–hexane	1.3439
384	3–iodo–5–methyl–hexane	1.3474
385	1–iodo–2,4–dimethyl–pentane	1.3611
386	2–iodo–2,4–dimethyl–pentane	1.3492
387	3–iodo–2,2–dimethyl–pentane	1.3559
388	3–iodo–2,4–dimethyl–pentane	1.3514
389	2–iodooctane	1.3026
390	3–iodooctane	1.3007
391	4–iodooctane	1.3001
392	2–iodo–6–methyl–heptane	1.3080

Table 7. (Continued)

No	RX	D_{pred} (g cm^{-3})
393	3–iodo–2–methyl–heptane	1.3044
394	4–iodo–4–methyl–heptane	1.3031
395	1–iodo–2,5–dimethyl–hexane	1.3179
396	2–iodo–2,3–dimethyl–hexane	1.3100
397	2–iodo–2,5–dimethyl–hexane	1.3074
398	3–iodo–2,2–dimethyl–hexane	1.3133
399	3–iodo–2,5–dimethyl–hexane	1.3096
400	3–iodo–3,5–dimethyl–hexane	1.3082
401	3–iodo–4,4–dimethyl–hexane	1.3175
402	1–iodo–2–ethyl–hexane	1.3140
403	methylamine	–
404	ethylamine	0.6996
405	propylamine	0.7211
406	isopropylamine	0.6918
407	butylamine	0.7394
408	sec–butylamine	0.7352
409	iso–butylamine	0.7415
410	tert–butylamine	0.7351
411	pentylamine	0.7548
412	1–methyl–butylamine	0.7509
413	1–ethyl–propylamine	0.7501
414	2,2–dimethyl–propylamine	0.7621
415	3–methyl–butylamine	0.7584
416	1,1–dimethyl–propylamine	0.7513
417	1,2–dimethyl–propylamine	0.7540
418	hexylamine	0.7674
419	1–methyl–pentylamine	0.7638
420	2–methyl–pentylamine	0.7703
421	3–methyl–pentylamine	0.7722
422	4–methyl–pentylamine	0.7713
423	1,2–dimethyl–butylamine	0.7680
424	1,3–dimethyl–propylamine	0.7676
425	1–isopropyl–propylamine	0.7663
426	1–ethyl–1–methyl–propylamine	0.7651
427	2,2–dimethyl–butylamine	0.7745
428	2,3–dimethyl–butylamine	0.7750
429	1,1,2–trimethyl–propylamine	0.7685
430	2–ethyl–butylamine	0.7712
431	heptylamine	0.7782
432	1–methyl–hexylamine	0.7749
433	1–propyl–butylamine	0.7737
434	2–methylhexylamine	0.7809
435	3–methyl–hexylamine	0.7831
436	4–methyl–hexylamine	0.7834
437	5–methyl–hexylamine	0.7819
438	1,1–dimethyl–pentylamine	0.7756
439	1,4–dimethyl–pentylamine	0.7786
440	1–isopropyl–butylamine	0.7770
441	1–ethyl–1–methyl–butylamine	0.7764
442	1–ethyl–3–methyl–butylamine	0.7775
443	2,4–dimethyl–pentylamine	0.7851
444	1,1,3–trimethyl–butylamine	0.7797
445	1–ethyl–2,2–dimethyl–propylamine	0.7836
446	1–isopropyl–2methyl–propylamine	0.7806
447	1–methyl–heptylamine	0.7842
448	1–ethyl–hexylamine	0.7833

Table 7. (Continued)

No	RX	D_{pred} (g cm^{-3})
449	1–propyl–pentylamine	0.7830
450	1,5–dimethyl–hexylamine	0.7878
451	1–isopropyl–pentylamine	0.7861
452	1–propyl–1–methyl–butylamine	0.7862
453	2,5–dimethyl–hexylamine	0.7937
454	1,1,2–trimethyl–pentylamine	0.7908
455	1,1,4–trimethyl–pentylamine	0.7887
456	1–tert–butyl–butylamine	0.7925
457	1–isopropyl–3–methyl–butylamine	0.7897
458	1–ethyl–1,3–dimethyl–butylamine	0.7897
459	1–ethyl–2,2–dimethyl–butylamine	0.7953
460	2–ethyl–hexylamine	0.7912
461	1,1–diethyl–butylamine	0.7874
462	1,1,3,3–tetramethyl–butylamine	0.7959
463	1–isopropyl–2,2–dimethyl–propylamin	0.7963
464	1–isopropyl–1,2–dimethyl–propylamine	0.7943
465	2–ethyl–1,1–dimethyl–butylamine	0.7925
466	1,1–diethyl–2–methyl–propylamine	0.7915
467	nonylamine	0.7951
468	1–methyl–octylamine	0.7923
469	1–ethyl–heptylamine	0.7915
470	1–propyl–hexylamine	0.7911
471	1–butyl–pentylamine	0.7910
472	1,1–dimethyl–heptylamine	0.7931
473	1–propyl–1–methyl–pentylamine	0.7944
474	1,1,5–trimethyl–hexylamine	0.8009
475	1–isopropyl–1–methyl–pentylamine	0.7975
476	1–isopropyl–4–methyl–pentylamine	0.8019
477	1–propyl–1,3–dimethyl–butylamine	0.7981
478	1–isobutyl–3–methyl–butylamine	0.8020
479	1–ethyl–1–propyl–butylamine	0.7962
480	2–ethyl–3–methyl–hexylamine	0.8054
481	1–tert–butyl–1–methyl–butylamine	0.8053
482	1–isopropyl–2,2–dimethyl–butylamine	0.8066
483	decylamine	0.8019
484	1–methyl–nonylamine	0.7993
485	1–propyl–heptyamine	0.7982
486	1–isopropyl–2,2–dimethyl–butylamine	0.8043
487	1–isobutyl–3–methyl–pentylamine	0.8059
488	1–isopropyl–1–ethyl–butylamine	0.8074
489	bromomethane	–
490	bromoethane	1.4607
491	1–bromopropane	1.3349
492	2–bromopropane	1.2931
493	1–bromobutane	1.2562
494	2–bromobutane	1.2493
495	1–bromo–2–methyl–propane	1.2594
496	2–bromo–2–methyl–propane	1.2486
497	1–bromopentane	1.2022
498	2–bromopentane	1.1960
499	3–bromopentane	1.1949
500	1–bromo–2,2–dimethyl–propane	1.2127
501	1–bromo–3–methyl–butane	1.2074
502	2–bromo–2–methyl–butane	1.1962
503	2–bromo–3–methyl–butane	1.2005
504	1–bromohexane	1.1624

Table 7. (Continued)

No	RX	D_{pred} (g cm^{-3})
505	2–bromohexane	1.1569
506	1–bromo–2–methyl–pentane	1.1664
507	1–bromo–3–methyl–pentane	1.1690
508	1–bromo–4–methyl–pentane	1.1679
509	2–bromo–3–methyl–pentane	1.1627
510	2–bromo–4–methyl–pentane	1.1621
511	3–bromo–2–methyl–pentane	1.1602
512	3–bromo–3–methyl–pentane	1.1581
513	1–bromo–2,2–dimethyl–butane	1.1721
514	1–bromo–2,3–dimethyl–butane	1.1728
515	2–bromo–2,3–dimethyl–butane	1.1630
516	1–bromo–2–ethyl–butane	1.1675
517	1–bromoheptane	1.1320
518	2–bromoheptane	1.1271
519	4–bromoheptane	1.1254
520	1–bromo–2–methyl–hexane	1.1357
521	1–bromo–3–methyl–hexane	1.1387
522	1–bromo–4–methyl–hexane	1.1391
523	1–bromo–5–methyl–hexane	1.1371
524	2–bromo–2–methyl–hexane	1.1278
525	2–bromo–5–methyl–hexane	1.1321
526	3–bromo–2–methyl–hexane	1.1298
527	3–bromo–3–methyl–hexane	1.1288
528	3–bromo–5–methyl–hexane	1.1306
529	1–bromo–2,4–dimethyl–pentane	1.1413
530	2–bromo–2,4–dimethyl–pentane	1.1332
531	3–bromo–2,2–dimethyl–pentane	1.1387
532	3–bromo–2,4–dimethyl–pentane	1.1347
533	2–bromooctane	1.1035
534	3–bromooctane	1.1022
535	4–bromooctane	1.1018
536	2–bromo–6–methyl–heptane	1.1083
537	3–bromo–2–methyl–heptane	1.1059
538	4–bromo–4–methyl–heptane	1.1057
539	1–bromo–2,5–dimethyl–hexane	1.1163
540	2–bromo–2,3–dimethyl–hexane	1.1118
541	2–bromo–2,5–dimethyl–hexane	1.1091
542	3–bromo–2,2–dimethyl–hexane	1.1142
543	3–bromo–2,5–dimethyl–hexane	1.1106
544	3–bromo–3,5–dimethyl–hexane	1.1103
545	3–bromo–4,4–dimethyl–hexane	1.1179
546	1–bromo–2–ethyl–hexane	1.1129
547	3–bromo–3–ethyl–hexane	1.1072
548	2–bromo–2,4,4–trimethyl–pentane	1.1185
549	3–bromo–2,2,4–trimethyl–pentane	1.1191
550	3–bromo–2,3,4–trimethyl–pentane	1.1163
551	2–bromo–3–ethyl–2–methyl–pentane	1.1140
552	3–bromo–3–ethyl–2–methyl–pentane	1.1126
553	1–bromononane	1.0884
554	2–bromononane	1.0844
555	3–bromononane	1.0832
556	4–bromononane	1.0828
557	5–bromononane	1.0826
558	2–bromo–2–methyl–octane	1.0852
559	4–bromo–4–methyl–octane	1.0867
560	2–bromo–2,6–dimethyl–heptane	1.0953

Table 7. (Continued)

No	RX	D_{pred} (g cm^{-3})
561	3–bromo–2,3–dimethyl–heptane	1.0906
562	3–bromo–2,6–dimethyl–heptane	1.0966
563	4–bromo–2,4–dimethyl–heptane	1.0914
564	4–bromo–2,6–dimethyl–heptane	1.0967
565	4–bromo–4–ethyl–heptane	1.0889
566	1–bromo–2–ethyl–3–methyl–hexane	1.1015
567	3–bromo–2,2,3–trimethyl–hexane	1.1007
568	3–bromo–2,4,4–trimethyl–hexane	1.1026
569	1–bromodecane	1.0722
570	2–bromodecane	1.0686
571	4–bromodecane	1.0670
572	3–bromo–2,7–dimethyl–octane	1.0747
573	4–bromo–2,6–dimethyl–octane	1.0767
574	3–bromo–3–ethyl–2–methyl–heptane	1.0782
575	3–iodo–3–ethyl–hexane	1.3045
576	2–iodo–2,4,4–trimethyl–pentane	1.3177
577	3–iodo–2,2,4–trimethyl–pentane	1.3185
578	3–iodo–2,3,4–trimethyl–pentane	1.3144
579	2–iodo–3–ethyl–2–methyl–pentane	1.3124
580	3–iodo–3–ethyl–2–methyl–pentane	1.3103
581	1–iodononane	1.2743
582	2–iodononane	1.2685
583	3–iodononane	1.2667
584	4–iodononane	1.2661
585	5–iodononane	1.2659
586	2–iodo–2–methyl–octane	1.2680
587	4–iodo–4–methyl–octane	1.2692
588	2–iodo–2,6–dimethyl–heptane	1.2792
589	3–iodo–2,3–dimethyl–heptane	1.2732
590	3–iodo–2,6–dimethyl–heptane	1.2811
591	4–iodo–2,4–dimethyl–heptane	1.2744
592	4–iodo–2,6–dimethyl–heptane	1.2814
593	4–iodo–4–ethyl–heptane	1.2713
594	1–iodo–2–ethyl–3–methyl–hexane	1.2881
595	3–iodo–2,2,3–trimethyl–hexane	1.2841
596	3–iodo–2,4,4–trimethyl–hexane	1.2871
597	1–iododecane	1.2450
598	2–iododecane	1.2397
599	4–iododecane	1.2374
600	3–iodo–2,7–dimethyl–octane	1.2458
601	4–iodo–2,6–dimethyl–octane	1.2479
602	3–iodo–3–ethyl–2–methyl–heptane	1.2481

4 CONCLUSIONS

The above results imply that densities can be calculated well by the perturbation theory for the monosubstituted alkanes. The models (Eq. (5) and Eq. (8)) are reliable for estimating the densities of alkanes RH and monosubstituted alkanes RX. Therefore Eq. (5) and Eq. (8) are suggested to calculate the densities for the alkanes and monosubstituted alkanes whose densities are not determined experimentally yet. The predicted densities of 160 alkanes (including 150 alkanes with 1–10 carbon atoms and 10 normal chain alkanes with 11–20 carbon atoms) and some

monosubstituted alkanes RX by Eq. (5) and Eq. (8) were listed in Table 6 and Table 7, respectively, which provide reference density data for chemical engineering and petrochemical industries.

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