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Prediction of the Acentric Factor of Organic Compounds with the Positional Distributive Contribution Method

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ABSTRACT: A new universal method was proposed for the prediction of properties of organic compounds, such as critical properties, normal boiling point, and the enthalpy of vaporization. In this study, the positional distributive contribution method is further extended for the prediction of the acentric factor ω of a variety of pure organic compounds. Comparison results between experimental and calculated data indicate that the new model could provide very satisfactory results. The overall average absolute error for the ω prediction of 477 organic compounds is 0.0252 with 5.72 % mean absolute relative deviation, which is compared to 0.0569 and 14.58 % with the Constantinou and Gani method. Also, a good prediction of the proposed method shown in our previous works and this work suggests that it is possible to use the same universal formula to predict not only T_c, P_c, V_c, Z_c, T_b, T_m, and $\Delta_{vap}H_b$ but also ω of organic compounds, which further demonstrates the universality, stability, and accuracy of our proposed method.

INTRODUCTION

The acentric factor ω is a parameter that was originally defined (shown as eq 1) by Pitzer[1] to improve the accuracy of corresponding state correlations for heavier and more complex compounds.

$$\omega = -\log_{10}[\lim_{(T/T_c=0.7)}(P_{vp}/P_c)] - 1.0 \quad (1)$$

Thus, using vapor pressure values, many reported ω values of pure compounds are calculated based on its definition.[2]

Also, there are some procedures to estimate an unknown acentric factor.[2−6] For instance, using a simpler two-parameter equation for the vapor pressure derived from Clapeyron equation, the Edmister correlation has been developed.[4] Later, Lee and Kesler[5] proposed a useful estimation technique for the acentric factor based on the normal boiling point, the critical pressure, and critical temperature. However, it should be noticed that the accuracy of these methods mainly depends on the accuracy of the input parameters; hence, the sensitivity of ω to errors of input information is very great. As a consequence, estimated property values will not yield accurate acentric factors.

Also, it is possible to directly estimate ω via group/bond/atom contribution methods.[7−13] Hoshino et al.[7] presented a method for alkanes using only the molecular structure. Hart and Peng[8] proposed another group-contribution technique for both hydrocarbons and nonhydrocarbons. Constantinou et al.[12] extended their second-order GC method to the estimation of the acentric factor for a wide range of substances from group contributions only. Investigations[2] have denoted that the Constantinou and Gani method can be used with some confidence. Very recently, Gharagheizi et al. proposed an artificial neural network group contribution (ANN-GC) method for the prediction of acentric factors of pure compounds.[13]

Recently, Wang et al.[14−17] proposed the positional distributive contribution method for the prediction of critical parameters, normal boiling point, melting point, and the enthalpy of vaporization of organic compounds with a similar framework, and the proposed method performed well both in accuracy and generality. Therefore, the purpose of this study was to determine whether our proposed positional distributive contribution method could be used directly for ω estimation. For this purpose, 477 organic compounds from literature were selected, and the performance of our new model had been compared with the method of Constantinou and Gani.[12]

METHOD PROPOSED IN THIS WORK

Experimental Data. To develop a comprehensive model for the prediction of the acentric factor that has a wide range of applicability, the data set should be large in the number of pure compounds and comprehensive in the diversity of chemical families. In this work, the DIPPR 801 database was used to provide the data set of the related experimental data.[18] A total of 477 compounds containing carbon, hydrogen, oxygen, nitrogen, chlorine, bromine, and sulfur were used for the determination of group contributions, which includes linear, branched alkanes and cycloalkanes (125), alkenes (61), aromatics (44), ketones and aldehydes (37), alcohols (48), acids (32), esters and ether oxides (57), bromochloroalkanes (12), amines and pyridines (37), and nitriles and alkane thiols (24). When all of the group contribution values have been determined, the recommended 477 experimental data were used to validate and evaluate the performance of our new method.

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Table 1. Position Group Contributions for the Prediction of ω[a]

group	A	group	A
C−(CH_3)(H)3	0.033218529	C−(S)(H)3	0.025413662
C−(CH_2)(H)3	−0.028419687	C−(C)(S)(H)2	0.046454351
C−(CH)(H)3	−0.026407303	C−(C)2(S)(H)	0.084758263
C−(C)(H)3	−0.008522945	C−(C)3(S)	0.04665853
C−(C)2(H)2	0.039154429	Cb−(N)	0.048798453
C−(C)3(H)	0.072671046	C−(N)(H)3	0.114132803
C−(C)4	0.055603658	C−(C)(N)(H)2	0.124283724
Cd−(H)(O)	1.552739749	C−(C)2(N)(H)	0.119776879
Cd−(H)2	−0.148634871	C−(C)(CN)(H)2	0.183688545
Cd−(C)(H)	0.212368135	C−(C)2(CN)(H)	0.218379674
C−(Cd)(C)(H)2	0.048986195	O−(Cb)(H)	1.009686828
C−(Cd)(H)3	−0.012865795	O−(CH_2)(H)	1.963367521
Cd−(C)2	0.33387531	O−(CH)(H)	2.109666568
C−(Cd)(C)2(H)	0.07973853	O−(C)(H)	2.000112695
Cd−(Cd)(H)	0.346278759	O−(C)2	1.006619073
Cd═Cd	0.130297218	O−(CO)(CH_3)	0.259055487
C−(Cd)(C)3	0.058164476	O−(CO)(CH_2)	0.373263264
C−(Cd)(0)(H)2	0.053909539	O−(CO)(CH)	0.408773267
C−(O−C)(H)3	−0.071516372	O−(Cd)(C)	−0.506302586
C−(O−CO)(H)3	−0.017237133	O−(CO)(H)	1.408177216
C−(CO)(H)3	0.190483803	N−(CH_3)(H)2	0.273485517
C−(C)(CO)(H)2	0.19057642	N−(CH_2)(H)2	0.104325808
C−(C)2(CO)(H)	0.245272526	N−(CH)(H)2	0.148678001
C−(C)3(CO)	0.186050389	N−(C)(H)2	0.637023344
C−(C)(O)(H)2	0.010102553	N−(cyclopenty)(H)2	−0.024720752
C−(C)2(O)(H)	0.054080667	N−(cyclohexy)(H)2	0.389786014
C−(C)3(O)	0.009586711	N−(C)2(H)	−0.154394898
C−(O)2(H)2	−0.072893827	N−(C)3	−1.177984332
CO−(CH_3)(O)	−0.56730101	N−(Cb)(H)2	0.950185338
CO−(CH_2)(O)	0.047242435	N−(Cb)(C)(H)	0.869749356
CO−(CH)(O)	−0.116424631	N−(Cb)(C)2	−0.691098047
CO−(C)(O)	−0.189348627	NI−(Cb)2	0.413905275
CO−(O)(H)	0.900941165	S−(C)(H)	−0.043494288
CO−(C)(H)	−0.207326317	Cl^-	0.095381909
CO−(C)2	−1.305592927	Br^-	0.155108392
C−(C)(Br)(H)2	0.017913926	ortho correction[b]	−0.028225604
C−(C)2(Br)(H)	0.039027653	meta correction[b]	−0.011007463
C−(C)(Cl)(H)2	0.015479668	cyclopentane correction	−0.156029517
C−(C)2(Cl)(H)	0.06767836	cyclohexane correction	−0.23217243
C−(C)3(Cl)	0.001367087	C_{ob}[c]	−0.024913528
C−(C)(Cl)2(H)	0.011610493	C_{mb}[c]	−0.029219287
Cb−(H)	0.005279216	C_{pb}[c]	−0.038079304
Cb−(C)	−0.20125448	cyclopropane correction	−0.091212184
C−(Cb)(H)3	0.09178058	>(CH)-position factor	0.002060027
C−(Cb)2(H)2	0.278336072	>(C)< position factor	0.001229505
C−(Cb)(C)(H)2	0.135135599	double bond position factor	−0.008564439
C−(Cb)(C)2(H)	0.147716473	hydroxyl position factor	−0.007090151
C−(Cb)(C)3	0.090942019	*trans* or *cis* structure	0.00049375
Cb−(O)	0.667251088	carbonyl position factor	−0.005663156
Cb−(COOH)	2.019573154	phenol position factor	0.003630537
Cb−(Cb)	1.636285018		

[a] Note: The first symbol represents the element that forms the center of the group. The symbols between parentheses represent the elements to which it is linked. Usual symbols are used to represent the elements in their normal valence state. Elements in other valence states are distinguished by using additional characters; furthermore, different symbols represent multiple bonded carbons, depending on the element at the other end of the multiple bond: Cd, carbon forming a double bond with another carbon; Cb, carbon involved in a benzene or a pyridine ring; CO, C═O group; CN, C≡N group; N_I, nitrogen of the imide (C═N−) function. Also used for the nitrogen of pyridine derivatives. The pyridine ring is considered as formed of five Cb and one N_I. *trans* or *cis* correction: *cis*-structure correction is 1, and *trans* structure is −1. [b] Ortho and meta corrections consider interactions between alkyl chains through a benzene ring. [c] Corrections for pyridines: C_{ob}, C_{mb}, and C_{pb} pyridine corrections take into account alkyl ligands in position ortho, meta, and para with respect to the N element, respectively.

Positional Distributive Contribution Method for Acentric Factor. In this work, the specific position of a group in the molecule was considered as the position factor (P_k). The acentric factor function is constructed by all groups' contribution as well as the position distribution factor. The position factors were used to take into account longer distance interactions, which could distinguish the overall isomer include *cis*- and *trans*- or *Z*- and *E*-structure of organic compounds for their thermodynamics properties. The molecule structures were described according to the International Union of Pure and Applied Chemistry (IUPAC) nominating method, and thus, the only P_k values could be obtained for the relevant positional correction factor. In our method, six position factors have been considered, such as the >(CH)-position factor, >(C)< position factor, double bond position factor, hydroxyl position factor, carbonyl position factor, and phenol position factor. For instance, in the case of 2,3,3,4-tetramethylpentane, according to the IUPAC nominating method, since the position of (CH) group is 2 and 4, respectively, then, the position correlation factor P is 6 (= 2 + 4). Also, the position of the (C) group is 3; hence, the position correlation factor P is 3.

Here, the position distribution function for ω estimation is expressed as eqs 2 and 3. This expression is similar in framework with our previous methods used for the prediction of the critical properties of organic compounds containing various functionalities.

$$\omega = 7.86948 + \sum_i A_i N_i + \sum_j A_j \tanh(N_j/N) + \sum_k A_k P_k - 7.62053 \exp(1/M) + 0.025051 \exp(1/N) \quad (2)$$

$$N = \sum_i N_i + \sum_j N_j \quad (3)$$

Parameter A_i or A_j stands for i or j group contributions, N_i for the number of each group that the carbon element forms in the

Table 2. Fully Predictive Estimations of Acentric Factor ω Using the Positional Distributive Contribution Method

compounds	CAS	ω_{exp}	ω_{pred}	D^a
ethane	74-84-0	0.0990	0.0990	0.0000
propane	74-98-6	0.1530	0.0914	0.0616
butane	106-97-8	0.2010	0.1703	0.0307
2-methylpropane	75-28-5	0.1770	0.1464	0.0306
pentane	109-66-0	0.2510	0.2338	0.0172
2-methylbutane	78-78-4	0.2290	0.2079	0.0211
2,2-dimethylpropane	463-82-1	0.1970	0.1972	−0.0002
hexane	110-54-3	0.2940	0.2894	0.0046
2-methylpentane	107-83-5	0.2790	0.2635	0.0155
3-methylpentane	96-14-0	0.2740	0.2635	0.0105
2,2-dimethylbutane	75-83-2	0.2330	0.2328	0.0002
2,3-dimethylbutane	79-29-8	0.2480	0.2396	0.0084
heptane	142-82-5	0.3500	0.3403	0.0097
2-methylhexane	591-76-4	0.3282	0.3144	0.0138
3-methylhexane	589-34-4	0.3216	0.3145	0.0071
3-ethylpentane	617-78-7	0.3094	0.3125	-0.0031
2,2-dimethylpentane	590-35-2	0.2879	0.2838	0.0041
2,3-dimethylpentane	565-59-3	0.2923	0.2886	0.0037
2,4-dimethylpentane	108-08-7	0.3018	0.2926	0.0092
3,3-dimethylpentane	562-49-2	0.2672	0.2651	0.0021
2,2,3-trimethylbutane	464-06-2	0.2504	0.2599	-0.0095
octane	111-65-9	0.3980	0.3884	0.0096
2-methylheptane	592-27-8	0.3772	0.3625	0.0147
3-methylheptane	589-81-1	0.3718	0.3626	0.0092
4-methylheptane	589-53-7	0.3706	0.3646	0.0060
3-ethylhexane	619-99-8	0.3628	0.3605	0.0023
2,2-dimethylhexane	590-73-8	0.3378	0.3319	0.0059
2,3-dimethylhexane	584-94-1	0.3472	0.3366	0.0106
2,4-dimethylhexane	589-43-5	0.3436	0.3387	0.0049
2,5-dimethylhexane	592-13-2	0.3576	0.3428	0.0148
3,3-dimethylhexane	563-16-6	0.3202	0.3132	0.0070
3,4-dimethylhexane	583-48-2	0.3381	0.3387	−0.0006
2-methyl-3-ethylpentane	609-26-7	0.3294	0.3346	−0.0052
3-methyl-3-ethylpentane	1067-08-9	0.3050	0.2933	0.0117
2,2,3-trimethylpentane	564-02-3	0.2970	0.3060	−0.0090
2,2,4-trimethylpentane	540-84-1	0.3031	0.3101	−0.0070
2,3,3-trimethylpentane	560-21-4	0.2903	0.2873	0.0030
2,3,4-trimethylpentane	565-75-3	0.3161	0.3148	0.0013
nonane	111-84-2	0.4490	0.4345	0.0145
2-methyloctane	3221-61-2	0.4212	0.4086	0.0126
3-methyloctane	2216-33-3	0.4123	0.4087	0.0036
4-methyloctane	2216-34-4	0.4129	0.4107	0.0022
3-ethylheptane	15869-80-4	0.4080	0.4067	0.0013
4-ethylheptane	2216-32-2		0.4087	
2,2-dimethylheptane	1071-26-7	0.3899	0.3780	0.0119
2,3-dimethylheptane	3074-71-3		0.3828	
2,4-dimethylheptane	2213-23-2		0.3848	
2,5-dimethylheptane	2216-30-0		0.3869	
2,6-dimethylheptane	1072-05-5	0.3927	0.3910	0.0017
3,3-dimethylheptane	4032-86-4		0.3581	
3,4-dimethylheptane	922-28-1		0.3849	
3,5-dimethylheptane	926-82-9		0.3869	
4,4-dimethylheptane	1068-19-5		0.3750	
3-ethyl-2-methylhexane			0.3807	

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Table 2. Continued

compounds	CAS	ω_{exp}	ω_{pred}	D^a
3-ethyl-3-methylhexane			0.3215	
3-ethyl-4-methylhexane			0.3849	
4-ethyl-2-methylhexane			0.3828	
2,2,3-trimethylhexane	16747-25-4	0.3320	0.3521	−0.0201
2,2,4-trimethylhexane	16747-26-5	0.3210	0.3542	−0.0332
2,2,5-trimethylhexane	3522-94-9	0.3567	0.3583	−0.0016
2,3,3-trimethylhexane	16747-28-7		0.3334	
2,3,4-trimethylhexane	921-47-1		0.3610	
2,3,5-trimethylhexane	1069-53-0		0.3630	
2,4,4-trimethylhexane	16747-30-1	0.3522	0.3346	0.0176
3,3,4-trimethylhexane	16747-31-2		0.3355	
3,3-diethylpentane	1067-20-5	0.3381	0.3276	0.0105
3-ethyl-2,2-dimethylpentane	16747-32-3	0.3353	0.3501	−0.0148
3-ethyl-2,3-dimethylpentane	16747-33-4		0.3135	
3-ethyl-2,4-dimethylpentane	1068-87-7	0.3530	0.3590	−0.0060
2,2,3,3-tetramethylpentane	7154-79-2	0.2800	0.3028	−0.0228
2,2,3,4-tetramethylpentane	1186-53-4	0.3106	0.3303	−0.0197
2,2,4,4-tetramethylpentane	1070-87-7	0.3159	0.3239	−0.0080
2,3,3,4-tetramethylpentane	16747-38-9	0.3130	0.3116	0.0014
decane	124-18-5	0.4890	0.4793	0.0097
2-methylnonane	871-83-0	0.4723	0.4534	0.0189
3-methylnonane	5911-04-6	0.4649	0.4534	0.0115
4-methylnonane	17301-94-9	0.4651	0.4555	0.0096
5-methylnonane	15869-85-9	0.4562	0.4575	−0.0013
3-ethyloctane	5881-17-4		0.4514	
4-ethyloctane	15869-86-0		0.4535	
2,2-dimethyloctane	15869-87-1	0.4288	0.4227	0.0061
2,3-dimethyloctane	7146-60-3	0.4327	0.4275	0.0052
2,4-dimethyloctane	4032-94-4	0.4345	0.4296	0.0049
2,5-dimethyloctane	15869-89-3	0.4403	0.4316	0.0087
2,6-dimethyloctane	2051-30-1	0.4386	0.4337	0.0049
2,7-dimethyloctane	1072-16-8	0.4420	0.4378	0.0042
3,3-dimethyloctane	4110-44-5		0.4041	
3,4-dimethyloctane	15869-92-8		0.4296	
3,5-dimethyloctane	15869-93-9		0.4317	
3,6-dimethyloctane	15869-94-0		0.4337	
4,4-dimethyloctane	15869-95-1		0.4053	
4,5-dimethyloctane	15869-96-2		0.4337	
4-propylheptane	3178-29-8		0.4535	
3-ethyl-2-methylheptane	14676-29-0		0.4255	
3-ethyl-3-methylheptane	17302-01-1		0.3842	
3-ethyl-4-methylheptane	17302-01-1		0.4276	
3-ethyl-5-methylheptane	52896-90-9		0.4297	
4-ethyl-2-methylheptane	52896-88-5		0.4276	
4-ethyl-3-methylheptane	52896-89-6		0.4276	
4-ethyl-4-methylheptane	17302-04-4		0.3854	
5-ethyl-2-methylheptane	13475-78-0		0.4296	
2,2,3-trimethylheptane	52896-92-1		0.4238	
2,2,4-trimethylheptane	14720-74-2		0.3989	
2,2,5-trimethylheptane	20291-95-6		0.4010	
2,2,6-trimethylheptane	1190-83-6		0.4051	
2,3,3-trimethylheptane	16747-28-7		0.3782	
2,3,4-trimethylheptane	52896-95-4		0.4037	
2,3,5-trimethylheptane	20278-85-7		0.4058	

Table 2. Continued

compounds	CAS	ω_{exp}	ω_{pred}	D^a
2,3,6-trimethylheptane	4032-93-3		0.4098	
2,4,4-trimethylheptane	4032-92-2		0.3794	
2,4,5-trimethylheptane	20278-84-6		0.4078	
2,4,6-trimethylheptane	2613-61-8		0.4119	
2,5,5-trimethylheptane	1189-99-7		0.3806	
3,3,4-trimethylheptane	20278-87-9		0.3803	
3,3,5-trimethylheptane	7154-80-5	0.3820	0.3823	−0.0003
3,4,4-trimethylheptane	20278-88-0		0.3794	
3,4,5-trimethylheptane	20278-89-1		0.4079	
3,4-diethylhexane	19398-77-7		0.4256	
3,3-diethylhexane	17302-02-2		0.3643	
3-ethyl-2,2-dimethylhexane	20291-91-2		0.3949	
3-ethyl-2,3-dimethylhexane	52897-00-4		0.3669	
3-ethyl-2,4-dimethylhexane	7220-26-0		0.4017	
3-ethyl-2,5-dimethylhexane	52897-04-8		0.4058	
3-ethyl-3,4-dimethylhexane	52897-06-0		0.3604	
4-ethyl-2,2-dimethylhexane	52896-99-8		0.3969	
4-ethyl-2,3-dimethylhexane	52897-01-5		0.4017	
4-ethyl-2,4-dimethylhexane	52897-03-7		0.3595	
4-ethyl-3,3-dimethylhexane	52897-05-9		0.3782	
2,2,3,3-tetramethylhexane	13475-81-5	0.3640	0.3475	0.0165
2,2,3,4-tetramethylhexane	52897-08-2		0.3731	
2,2,3,5-tetramethylhexane	52897-09-3		0.3771	
2,2,4,4-tetramethylhexane	51750-65-3		0.3487	
2,2,5,5-tetramethylhexane	1071-81-4	0.3750	0.3699	0.0051
2,2,4,5-tetramethylhexane	16747-42-5		0.3792	
2,3,3,4-tetramethylhexane	52897-10-6		0.3543	
2,3,3,5-tetramethylhexane	52897-11-7		0.3584	
2,3,4,4-tetramethylhexane	52897-12-8		0.3535	
2,3,4,5-tetramethylhexane	52897-15-1		0.3840	
3,3,4,4-tetramethylhexane	5171-84-6		0.3301	
3,3-diethyl-2-methylpentane			0.3384	
3-ethyl-2,2,3-trimethylpentane	52897-17-3		0.2740	
3-ethyl-2,2,4-trimethylpentane	52897-18-4		0.3731	
3-ethyl-2,3,4-trimethylpentane	52897-19-5		0.3365	
2,2,3,3,4-pentamethylpentane	16747-44-7		0.3237	
2,2,3,4,4-pentamethylpentane	16747-45-8		0.3428	
undecane	1120-21-4	0.5320	0.5230	0.0090
2-methyldecane	6975-98-0		0.4971	
3-methyldecane	13151-34-3		0.4972	
4-methyldecane	2847-72-5		0.4992	
5-methyldecane	13151-35-4		0.5013	
2,3-dimethylnonane	2884-06-2		0.4712	
dodecane	112-40-3	0.5730	0.5660	0.0070
2-methylundecane	7045-71-8		0.5401	
3-methylundecane	1002-43-3	0.5516	0.5401	0.0114
4-methylundecane	2980-69-0		0.5422	
5-methylundecane	1632-70-8		0.5443	
2.3-dimethyldecane			0.5142	
2.4-dimethyldecane			0.5163	
3,3,6,6-tetramethyloctane	62199-46-6		0.4193	
2,2,4,6,6-pentamethylheptane	13475-82-6		0.4340	
tridecane	629-50-5	0.6230	0.6084	0.0146
2-methyldodecane	1560-97-0		0.5825	

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Table 2. Continued

compounds	CAS	ω_{exp}	ω_{pred}	D^a
3-methyldodecane	17312-57-1		0.5826	
4-methyldodecane	6117-97-1		0.5846	
5-methyldodecane	17453-93-9		0.5867	
2.3-dimethylundecane			0.5566	
2.4-dimethylundecane			0.5587	
4,4,6,6-tetramethylnonane	74286-93-4		0.4629	
2,5-dimethyl-3,5-diethylheptane			0.4620	
tetradecane	629-59-4	0.6670	0.6504	0.0166
2-methyltridecane	1560-96-9		0.6244	
3-methyltridecane	6418-41-3		0.6245	
4-methyltridecane	26730-12-1		0.6266	
5-methyltridecane	25117-31-1		0.6286	
7-methyltridecane	26730-14-3		0.6327	
2,3-dimethyldodecane	6117-98-2		0.5986	
2,4-dimethyldodecane	6117-99-3		0.6006	
pentadecane	629-62-9	0.7070	0.6919	0.0151
2-methyltetradecane	1560-95-8		0.6660	
3-methyltetradecane	18435-22-8		0.6661	
4-methyltetradecane	25117-24-2		0.6681	
5-methyltetradecane	25117-32-2		0.6702	
2,3-dimethyltridecane	18435-20-6		0.6402	
2,4-dimethyltridecane			0.6422	
2,4,6-trimethyldodecane			0.6225	
hexadecane	544-76-3	0.7440	0.7332	0.0108
2-methylpentadecane	1560-93-6		0.7073	
3-methylpentadecane	2882-96-4		0.7073	
4-methylpentadecane	2801-87-8		0.7094	
5-methylpentadecane	25117-33-3		0.7115	
2,3-dimethyltetradecane	18435-23-9		0.6814	
2,4-dimethyltetradecane			0.6835	
2,4,6-trimethyltridecane			0.6638	
heptadecane	629-78-7	0.7700	0.7742	−0.0042
2-methylhexadecane	1560-92-5		0.7483	
3-methylhexadecane	6418-43-5		0.7484	
4-methylhexadecane	25117-26-4		0.7504	
5-methylhexadecane			0.7525	
2,3-dimethylpentadecane	2882-97-5		0.7225	
2,4-dimethylpentadecane			0.7245	
2,4,6-trimethyltetradecane			0.7048	
octadecane	593-45-3	0.7951	0.8151	−0.0200
2-methylheptadecane	1560-89-0		0.7891	
3-methylheptadecane	6418-44-6		0.7892	
4-methylheptadecane	26429-11-8		0.7913	
5-methylheptadecane			0.7933	
2,3-dimethylhexadecane			0.7633	
2,4-dimethylhexadecane			0.7653	
2,4,6-trimethylpentadecane			0.7457	
nonadecane	629-92-5	0.8196	0.8557	−0.0361
2-methyloctadecane	1560-88-9		0.8298	
3-methyloctadecane	6561-44-0		0.8298	
4-methyloctadecane	10544-95-3		0.8319	
5-methyloctadecane	25117-35-5		0.8340	
2,3-dimethylheptadecane	61868-03-9		0.8039	
2,4-dimethylheptadecane			0.8060	

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Table 2. Continued

compounds	CAS	ω_{exp}	ω_{pred}	D^a
2,4,4-trimethylhexadecane			0.7863	
eicosane	112-95-8	0.8764	0.8962	−0.0198
2-methylnonadecane	1560-86-7		0.8703	
3-methylnonadecane	6418-45-7		0.8703	
4-methylnonadecane	25117-27-5		0.8724	
5-methylnonadecane			0.8745	
2,3-dimethyloctadecane			0.8444	
2,4-dimethyloctadecane			0.8465	
2,4,5-trimethylheptadecane			0.8268	
heneicosane	629-94-7	0.9420	0.9366	0.0054
2-methyleicosane	1560-84-5		0.9107	
docosane	629-97-0	0.9722	0.9768	−0.0046
tricosane	638-67-5	1.0262	1.0170	0.0092
tetracosane	646- 31-1	1.0710	1.0571	0.0139
pentacosane	629-99-2	1.1053	1.0971	0.0082
hexacosane	630-01-3	1.1544	1.1370	0.0174
heptacosane	593-49-7	1.2136	1.1769	0.0366
octacosane	630-02-4	1.2375	1.2168	0.0207
nonacosane	630-03-5	1.2653	1.2565	0.0088
triacontane	638-68-6	1.3072	1.2963	0.0109
untriacontane			1.3360	
dotriacontane	544-85-4	1.3765	1.3757	0.0008
tritriacontane	630-05-7		1.4153	
tetratriacontane	14167-59-0		1.4549	
pentatriacontane	630-07-9		1.4945	
hexatriacontane	630-06-8	1.5260	1.5341	−0.0081
tetracontane	4181-95-7		1.6921	
cyclopropane	75-19-4	0.1269	0.1269	0.0000
cyclobutane	287-23-0	0.1847	0.3007	−0.1160
cyclopentane	287-92-3	0.1960	0.2099	−0.0139
methylcyclopentane	96-37-7	0.2310	0.2364	−0.0054
ethylcyclopentane	1640-89-7	0.2710	0.2859	−0.0149
propylcyclopentane	2040-96-2	0.2719	0.3343	−0.0624
butylcyclopentane	2040-95-1	0.3719	0.3807	−0.0088
pentylcyclopentane	3741-00-2		0.4256	
hexylcyclopentane	4457-00-5	0.4760	0.4695	0.0065
heptylcyclopentane	5617-42-5	0.5150	0.5126	0.0024
octylcyclopentane	1795-20-6	0.5640	0.5551	0.0089
nonylcyclopentane	2882-98-6	0.6100	0.5971	0.0129
decylcyclopentane	1795-21-7	0.6540	0.6387	0.0153
undecylcyclopentane	6785-23-5		0.6800	
dodecylcyclopentane	5634-30-0	0.7190	0.7211	−0.0021
tridecylcyclopentane	6006-34-4	0.7550	0.7619	−0.0069
cis-1,2-dimethylcyclopentane	1192-18-3	0.2662	0.2605	0.0057
trans-1,2-dimethylcyclopentane	822-50-4	0.2698	0.2595	0.0103
cis-1,3-dimethylcyclopentane	2532-58-3	0.2743	0.2625	0.0118
trans-1,3-dimethylcyclopentane	1759-58-6	0.2699	0.2615	0.0084
1,1-dimethylcyclopentane	1638-26-2	0.2724	0.2402	0.0322
cyclohexane	110-82-7	0.2100	0.1902	0.0198
methylcyclohexane	108-87-2	0.2390	0.2118	0.0272
ethylcyclohexane	1678-91-7	0.2500	0.2582	−0.0082
propylcyclohexane	1678-92-8	0.2595	0.3046	−0.0451
butylcyclohexane	1678-93-9	0.2743	0.3495	−0.0752
pentylcyclohexane	4292-92-6		0.3934	

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Table 2. Continued

compounds	CAS	ω_{exp}	ω_{pred}	D^a
hexylcyclohexane	4292-75-5		0.4365	
heptylcyclohexane	5617-41-4		0.4789	
octylcyclohexane	1795-15-9		0.5209	
nonylcyclohexane	2883-02-5		0.5626	
decylcyclohexane	1795-16-0	0.6627	0.6039	0.0588
nonylcyclohexane	2883-02-5		0.6449	
dodecylcyclohexane	1795-17-1		0.6858	
1,1-dimethylcyclohexane	590-66-9	0.2326	0.2125	0.0201
cis-1,2-dimethylcyclohexane	2207-01-4	0.2324	0.2328	−0.0004
trans-1,2-dimethylcyclohexane	6876-23-9	0.2379	0.2318	0.0061
cis-1,3-dimethylcyclohexane	638-04-0	0.2366	0.2348	0.0018
trans-1,3-dimethylcyclohexane	2207-03-6	0.2335	0.2338	−0.0003
cis-1,4-dimethylcyclohexane	624-29-3	0.2311	0.2369	−0.0058
trans-1,4-dimethylcyclohexane	2207-04-7	0.2370	0.2359	0.0011
1-butene	106-98-9	0.1910	0.1717	0.0193
cis-2-butene	590-18-1	0.2020	0.1998	0.0022
trans-2-butene	624-64-6	0.2190	0.1989	0.0201
1-pentene	109-67-1	0.2940	0.2338	0.0602
cis-2-pentene	627-20-3	0.2380	0.2419	−0.0039
trans-2-pentene	646-04-8	0.2373	0.2409	−0.0036
2-methyl-1-butene	563-46-2	0.2340	0.2083	0.0257
2-methyl-2-butene	513-35-9	0.2490	0.2247	0.0243
3-methyl-1-butene	563-45-1	0.2340	0.2072	0.0268
1-hexene	592-41-6	0.2960	0.2883	0.0077
cis-2-hexene	7688-21-3	0.2722	0.2860	−0.0138
trans-2-hexene	4050-45-7	0.2613	0.2850	−0.0237
cis-3-hexene	7642-09-3	0.2787	0.2717	0.0070
trans-3-hexene	13269-52-8	0.2854	0.2707	0.0147
2-methyl-1-pentene	763-29-1	0.2406	0.2588	−0.0182
3-methyl-1-pentene	760-20-3	0.2640	0.2597	0.0043
4-methyl-1-pentene	691-37-2	0.2389	0.2665	−0.0276
3-methyl-*cis*-2-pentene	922-62-3	0.2585	0.2596	−0.0011
3-methyl-*trans*-2-pentene	616-12-6	0.2627	0.2586	0.0041
4-methyl-*cis*-2-pentene	691-38-3	0.2442	0.2614	−0.0172
4-methyl-*trans*-2-pentene	674-76-0	0.2552	0.2604	−0.0052
2-methyl-2-pentene	625-27-4	0.2445	0.2578	−0.0133
2,3-dimethyl-1-butene	563-78-0	0.2333	0.2322	0.0011
3,3-dimethyl-1-butene	558-37-2	0.2257	0.2257	0.0000
2,3-dimethyl-2-butene	563-79-1	0.2237	0.2348	−0.0111
1-heptene	592-76-7	0.3310	0.3383	−0.0073
cis-2-heptene	6443-92-1	0.2942	0.3283	−0.0341
trans-2-heptene	14686-13-6	0.3372	0.3273	0.0099
cis-3-heptene	7642-10-6	0.2949	0.3140	−0.0191
trans-3-heptene	14686-14-7	0.3341	0.3130	0.0211
2-methyl-1-hexene	6094-02-6	0.3094	0.3060	0.0034
3-methyl-1-hexene	3404-61-3	0.3057	0.3097	−0.0040
4-methyl-1-hexene	3769-23-1	0.3024	0.3166	−0.0142
5-methyl-1-hexene	3524-73-0	0.3105	0.3186	−0.0082
3-methyl-*cis*-2-hexene	10574-36-4		0.2984	
3-methyl-*trans*-2-hexene			0.2974	
4-methyl-*cis*-2-hexene	3683-19-0		0.3017	
4-methyl-*trans*-2-hexene	3683-22-5		0.3007	
5-methyl-*cis*-2-hexene			0.3086	
5-methyl-*trans*-2-hexene	7385-82-2		0.3076	

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Table 2. Continued

compounds	CAS	ω_{exp}	ω_{pred}	D^a
2-methyl-*cis*-3-hexene			0.2853	
2-methyl-*trans*-3-hexene	692-24-0		0.2843	
3-methyl-*cis*-3-hexene	4914-89-0		0.2841	
3-methyl-*trans*-3-hexene	3899-36-3		0.2831	
2-ethyl-1-pentene	3404-71-5	0.3073	0.3003	0.0070
3-ethyl-1-pentene	4038-04-4	0.3019	0.3077	−0.0058
2,3-dimethyl-1-pentene	3404-72-6		0.2774	
2,4-dimethyl-1-pentene	2213-32-3		0.2842	
3,3-dimethyl-1-pentene	3404-73-7		0.3098	
3,4-dimethyl-1-pentene	7385-78-6		0.2879	
4,4-dimethyl-1-pentene	762-62-9		0.2843	
3-ethyl-2-pentene	816-79-5		0.2922	
2,3-dimethyl-2-pentene	10574-37-5		0.2637	
2,4-dimethyl-2-pentene	625-65-0		0.2721	
3,4-dimethyl-*cis*-2-pentene	4914-91-4		0.2738	
3,4-dimethyl-*trans*-2-pentene	4914-92-5		0.2728	
4,4-dimethyl-*cis*-2-pentene	762-63-0		0.2669	
4,4-dimethyl-*trans*-2-pentene	690-08-4		0.2659	
1-octene	111-66-0	0.3747	0.3857	−0.0110
cis-2-octene	7642-04-8	0.3889	0.3697	0.0192
trans-2-octene	13389-42-9	0.3384	0.3687	−0.0303
cis-3-octene	14850-22-7	0.3800	0.3554	0.0246
trans-3-octene	14919-01-8	0.3438	0.3544	−0.0106
cis-4-octene	7642-15-1	0.3854	0.3468	0.0386
trans-4-octene	14850-23-8	0.3393	0.3458	−0.0065
1-nonene	124-11-8	0.4171	0.4312	−0.0141
1-decene	872-05-9	0.4645	0.4754	−0.0109
cis-5-decene	7433-78-5		0.4905	
trans-5-decene	7433-56-9		0.4185	
1-undecene	821-95-4	0.5171	0.5187	−0.0016
cis-2-undecene	821-96-5		0.4904	
trans-2-undecene	693-61-8		0.4894	
cis-3-undecene	821-97-6		0.4767	
trans-3-undecene	1002-68-2		0.4757	
cis-4-undecene	821-98-7		0.4682	
trans-4-undecene	693-62-9		0.4672	
cis-5-undecene	764-96-5		0.4596	
trans-5-undecene	764-97-6		0.4586	
1-dodecene	112-41-4	0.5705	0.5613	0.0092
1-tridecene	2437-56-1	0.6063	0.6034	0.0029
1-tetradecene	1120-36-1	0.6449	0.6450	−0.0001
1-pentadecene	13360-61-7	0.6837	0.6864	−0.0027
1-hexadecene	629-73-2	0.7242	0.7274	−0.0032
1-heptadecene	6765-39-5	0.7527	0.7682	−0.0155
1-octadecene	112-88-9	0.7943	0.8089	−0.0146
1-nonadecene	18435-45-5	0.8409	0.8494	−0.0085
1-eicosene	3452-07-1	0.8804	0.8897	−0.0093
1,2-butadiene	590-19-2	0.1659	0.1449	0.0210
1,3-butadiene	106-99-0	0.1960	0.1960	0.0000
1,2-pentadiene	591-95-7	0.1542	0.2000	−0.0458
1,(*Z*)3-pentadiene			0.2644	
1,(*E*)3-pentadiene			0.2634	
2,3-pentadiene	591-96-8	0.2184	0.2047	0.0137
3-methyl-1,2-butadiene	598-25-4	0.1874	0.1814	0.0060

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Table 2. Continued

compounds	CAS	ω_{exp}	ω_{pred}	D^a
2-methyl-1,3-butadiene	78-79-5	0.1510	0.1735	−0.0225
benzene	71-43-2	0.2103	0.1844	0.0259
methylbenzene	108-88-3	0.2640	0.2612	0.0028
1,4-dimethylbenzene	106-42-3	0.3218	0.3419	−0.0201
1,2-dimethylbenzene	95-47-6	0.3101	0.3137	−0.0036
1,3-dimethylbenzene	108-38-3	0.3265	0.3309	−0.0044
ethylbenzene	100-41-4	0.3035	0.2898	0.0137
1,2,3-trimethylbenzene	526-73-8	0.3666	0.3582	0.0084
1,2,4-trimethylbenzene	95-63-6	0.3787	0.3864	−0.0077
1,3,5-trimethylbenzene	108-67-8	0.3985	0.3926	0.0059
1,2,3,4-tetramethylbenzene	488-23-3	0.4172	0.4047	0.0125
1,2,3,5-tetramethylbenzene	527-53-7	0.4242	0.4219	0.0023
1,2,4,5-tetramethylbenzene	95-93-2	0.4217	0.4329	−0.0112
1-methyl-2-ethylbenzene	611-14-3	0.3353	0.3417	−0.0064
1-methyl-3-ethylbenzene	620-14-4	0.3649	0.3590	0.0059
1-methyl-4-ethylbenzene	622-96-8	0.3666	0.3700	−0.0034
propylbenzene	103-65-1	0.3444	0.3395	0.0049
isopropylbenzene	98-82-8	0.3274	0.2886	0.0388
1-methyl-2-isopropylbenzene	527-84-4	0.3662	0.3404	0.0258
1-methyl-3-isopropylbenzene	535-77-3	0.3780	0.3576	0.0204
1-methyl-4-isopropylbenzene	99-87-6	0.3738	0.3686	0.0052
1-methyl-2-propylbenzene	1074-17-5	0.407	0.3914	0.0156
1-methyl-3-propylbenzene	1074-43-7	0.4128	0.4086	0.0042
1-methyl-4-propylbenzene	1074-55-1	0.4134	0.4196	−0.0062
butylbenzene	104-51-8	0.3941	0.3871	0.0070
sec-butylbenzene	135-98-8	0.2791	0.3341	−0.0550
tert-butylbenzene	98-06-6	0.2674	0.2674	0.0000
pentylbenzene	538-68-1	0.4388	0.4330	0.0058
hexylbenzene	1077-16-3	0.4790	0.4778	0.0012
heptylbenzene	1078-71-3	0.5287	0.5216	0.0071
1,2-diethylbenzene	135-01-3	0.3395	0.3671	−0.0276
1,3-diethylbenzene	141-93-5	0.3540	0.3844	−0.0304
1,4-diethylbenzene	105-05-5	0.4028	0.3954	0.0074
1,2-dimethyl-3-ethylbenzene	933-98-2	0.3621	0.3854	−0.0233
1,2-dimethyl-4-ethylbenzene	934-80-5	0.4114	0.4136	−0.0022
1,3-dimethyl-2-ethylbenzene	2870-04-4	0.4066	0.3854	0.0212
1,3-dimethyl-4-ethylbenzene	874-41-9	0.4140	0.4136	0.0004
1,3-dimethyl-5-ethylbenzene	934-74-7	0.4169	0.4198	−0.0029
1,4-dimethyl-2-ethylbenzene	1758-88-9	0.4114	0.4136	−0.0022
1,2-diisopropylbenzene	577-55-9		0.3591	
1,3-diisopropylbenzene	99-62-7	0.3587	0.3763	−0.0176
diphenylmethane	101-81-5	0.4816	0.4816	0.0000
biphenyl	92-52-4	0.4029	0.5004	−0.0975
o-terphenyl	84-15-1	0.5513	0.5752	−0.0239
m-terphenyl	92-06-8	0.6509	0.5925	0.0584
p-terphenyl	92-94-4	0.6426	0.6035	0.0391
butanone	78-93-3	0.3241	0.1962	0.1279
2-pentanone	107-87-9	0.3456	0.3133	0.0323
3-pentanone	96-22-0	0.3448	0.2402	0.1046
2-methylcyclopentanone	1120-72-5		0.3162	
3-methylcyclopentanone	1757-42-2/ 6672-30-6		0.3183	
2-propylcyclopentanone	1193-70-0		0.4604	
3-methyl-2-butanone	563-80-4	0.3208	0.3107	0.0101
2-hexanone	591-78-6	0.3846	0.4061	−0.0215

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Table 2. Continued

compounds	CAS	ω_{exp}	ω_{pred}	D^a
3-hexanone	589-38-8	0.3801	0.3330	0.0471
3,3-dimethyl-2-butanone	75-97-8	0.3298	0.3298	0.0000
3-methyl-2-pentanone	565-61-7	0.3854	0.4014	−0.0160
4-methyl-2-pentanone	108-10-1	0.3557	0.3843	−0.0286
2-methyl-3-pentanone	565-69-5	0.3891	0.3282	0.0609
2-heptanone	110-43-0	0.4190	0.4843	−0.0653
3-heptanone	106-35-4	0.4076	0.4112	−0.0036
4-heptanone	123-19-3	0.4120	0.4055	0.0065
5-methyl-2-hexanone	110-12-3	0.4344	0.4646	−0.0302
2-methyl-3-hexanone	7379-12-6		0.4065	
2,2-dimethyl-3-pentanone	564-04-5		0.3337	
2,4-dimethyl-3-pentanone	565-80-0	0.4053	0.4058	−0.0005
2-octanone	111-13-7	0.4549	0.5532	−0.0983
3-octanone	106-68-3	0.4406	0.4801	−0.0395
4-octanone	589-63-9	0.4204	0.4744	−0.0540
2-methyl-3-heptanone	13019-20-0		0.4754	
5-methyl-3-heptanone	541-85-5		0.4584	
2,2,4-trimethyl-3-pentanone	5857-36-3		0.4020	
5-nonanone	502-56-7	0.5137	0.6158	−0.1021
4-nonanone	4485-09-0	0.4988	0.5426	−0.0438
3-nonanone	925-78-0	0.4629	0.5370	−0.0741
2-nonanone	821-55-6	0.4979	0.5313	−0.0334
2,6-dimethyl-4-heptanone	108-83-8	0.5116	0.4934	0.0182
2 decanone	693-54-9		0.6738	
3 decanone	928-80-3		0.6007	
4 decanone	624-16-8		0.5950	
5 decanone	820-29-1		0.5894	
2-undecanone	112-12-9		0.7285	
3-undecanone	2216-87-7		0.6554	
4-undecanone	14476-37-0		0.6497	
5-undecanone	33083-83-9		0.6441	
6-undecanone	927-49-1	0.5928	0.6384	−0.0456
2-dodecanone	6175-49-1		0.7807	
3-dodecanone	1534-27-6		0.7076	
4-dodecanone	6137-26-4		0.7019	
5-dodecanone	19780-10-0		0.6963	
6-dodecanone	6064-27-3		0.6906	
2-tridecanone	593-08-8		0.8310	
3-tridecanone	1534-26-5		0.7578	
4-tridecanone	26215-90-7		0.7521	
5-tridecanone	30692-16-1		0.7465	
6-tridecanone	22026-12-6		0.7408	
7-tridecanone	462-18-0		0.7352	
2-tetradecanone	2345-27-9		0.8796	
3-tetradecanone	629-23-2		0.8065	
4-tetradecanone	26496-20-8		0.8008	
7-tetradecanone	6137-34-4		0.7839	
2-pentadecanone	2345-28-0		0.9271	
8-pentadecanone	818-23-5		0.8256	
2-hexadecanone	18787-63-8		0.9735	
2-heptadecanone	2922-51-2		1.0191	
9-heptadecanone	540-08-9		0.9120	
propanal	123-38-6	0.2559	0.2414	0.0145
butanal	123-72-8	0.2774	0.3196	−0.0422

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Table 2. Continued

compounds	CAS	ω_{exp}	ω_{pred}	D^a
2 methylpropanal	78-84-2	0.3622	0.3148	0.0474
1-pentanal	110-62-3	0.3472	0.3844	−0.0372
1-hexanal	66-25-1	0.4390	0.4418	−0.0028
1-heptanal	111-71-7	0.4865	0.4945	−0.0080
1-octanal	124-13-0	0.5471	0.5442	0.0029
1-nonanal	124-19-6	0.5920	0.5917	0.0003
1-decanal	112-31-2	0.6416	0.6376	0.0040
undecanal	112-44-7	0.6966	0.6824	0.0142
dodecanal	112-54-9	0.7538	0.7264	0.0274
tetradecanal	124-25-4		0.8123	
hexadecanal	629-80-1		0.8964	
2-methylhexanal	952-54-2	0.4637	0.4686	−0.0049
3-methylhexanal	19269-28-4	0.4640	0.4686	−0.0046
ethanol	64-17-5	0.6452	0.7225	−0.0773
1-propanol	71-23-8	0.6218	0.6479	−0.0261
2-propanol	67-63-0	0.6689	0.6612	0.0077
1-butanol	71-36-3	0.5935	0.6165	−0.0230
2-butanol	78-92-2	0.5722	0.6208	−0.0486
2-methyl-1-propanol	78-83-1	0.5848	0.5926	−0.0078
2-methyl-2-propanol	75-65-0	0.6115	0.5431	0.0684
1-pentanol	71-41-0	0.5938	0.6079	−0.0141
2-pentanol	6032-29-7	0.6746	0.6075	0.0671
3-pentanol	584-02-1	0.6748	0.6005	0.0743
2-methyl-1-butanol	137-32-6	0.6784	0.5800	0.0984
3-methyl-1-butanol	123-51-3	0.5558	0.5840	−0.0282
2-methyl-2-butanol	75-85-4	0.4831	0.5135	−0.0304
3-methyl-2-butanol	598-75-4	0.3510	0.5836	−0.2326
1-hexanol	111-27-3	0.5791	0.6127	−0.0336
2-hexanol	626-93-7	0.5655	0.6089	−0.0434
3-hexanol	623-37-0		0.6019	
2-methyl-1-pentanol	105-30-6	0.7262	0.5848	0.1414
3-methyl-1-pentanol	589-35-5	0.7230	0.5868	0.1362
4-methyl-1-pentanol	626-89-1		0.5909	
2-methyl-2-pentanol	590-36-3		0.5174	
3-methyl-2-pentanol	565-60-6		0.5830	
4-methyl-2-pentanol	108-11-2	0.5723	0.5871	−0.0148
2-methyl-3-pentanol	565-67-3		0.5759	
3-methyl-3-pentanol	77-74-7	0.4318	0.4917	−0.0598
2-ethyl-1-butanol	97-95-0	0.7136	0.5828	0.1308
2,2-dimethyl-1-butanol	1185-33-7		0.5363	
3,3-dimethyl-1-butanol	624-95-3		0.5574	
2,3-dimethyl-2-butanol	594-60-5		0.5408	
3,3-dimethyl-2-butanol	464-07-3		0.5536	
1-heptanol	111-70-6	0.5874	0.6260	−0.0386
2-heptanol	543-49-7	0.7627	0.6125	0.1502
3-heptanol	589-82-2		0.6126	
4-heptanol	589-55-9		0.6076	
1-octanol	111-87-5	0.5941	0.6450	−0.0509
2-octanol	123-96-6	0.5056	0.6366	−0.1310
3-octanol	589-98-0/20296-29-1		0.6296	
4-octanol	589-62-8		0.6245	
2-methyl-1-heptanol	60435-70-3		0.6171	
3-methyl-1-heptanol	1070-32-2		0.6191	
4-methyl-1-heptanol	817-91-4		0.6232	

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Table 2. Continued

compounds	CAS	ω_{exp}	ω_{pred}	D^a
5-methyl-1-heptanol	7212-53-5		0.4084	
2-methyl-2-heptanol	625-25-2		0.5485	
3-methyl-2-heptanol	31367-46-1		0.6108	
4-methyl-2-heptanol	56298-90-9		0.6128	
5-methyl-2-heptanol	54630-50-1		0.6149	
6-methyl-2-heptanol	4730-22-7/67952-57-2		0.6169	
2-methyl-3-heptanol	18720-62-2		0.6037	
3-methyl-3-heptanol	5582-82-1		0.5228	
4-methyl-3-heptanol	14979-39-6	0.5800	0.6058	−0.0258
5-methyl-3-heptanol	18720-65-5	0.5870	0.6078	−0.0208
6-methyl-3-heptanol	18720-66-6		0.6099	
2-methyl-4-heptanol	21570-35-4		0.5986	
4-methyl-4-heptanol	598-01-6		0.5169	
2,2-dimethyl-1-hexanol	2370-13-0		0.5685	
2-ethyl-1-hexanol	104-76-7	0.549	0.6150	−0.0660
1-nonanol	143-08-8	0.6267	0.6680	−0.0413
2-nonanol	70419-06-6	0.8904	0.6580	0.2324
3-nonanol	624-51-1		0.6510	
4-nonanol	5932-79-6		0.6459	
5-nonanol	623-93-8		0.6409	
1-decanol	112-30-1	0.6612	0.6939	−0.0327
2-decanol	1120-06-5		0.6826	
3-decanol	1565-81-7		0.6756	
4-decanol	2051-31-2		0.6705	
5-decanol	5205-34-5		0.6655	
1-undecanol	112-42-5	0.6100	0.7220	−0.1120
2-undecanol	1653-30-1		0.7097	
3-undecanol	6929-08-4		0.7026	
6-undecanol	23708-56-7		0.6875	
1-dodecanol	112-53-8	0.6664	0.7519	−0.0855
2-dodecanol	10203-28-8		0.7385	
3-dodecanol	10203-30-2		0.7315	
1-tridecanol	112-70-9	0.7124	0.7830	−0.0706
2-tridecanol	1653-31-2		0.7689	
3-tridecanol	10289-68-6		0.7619	
1-tetradecanol	112-72-1	0.7432	0.8152	−0.0720
3-tetradecanol	1653-32-3		0.7934	
1-pentadecanol	629-76-5	0.7797	0.8483	−0.0686
3-pentadecanol			0.8259	
phenol	108-95-2	0.4259	0.4376	−0.0117
o-cresol	95-48-7	0.4335	0.4633	−0.0298
m-cresol	108-39-4	0.4493	0.4841	−0.0348
p-cresol	106-44-5	0.5134	0.4988	0.0146
2,3-xylenol	526-75-0	0.5157	0.4918	0.0239
2,4-xylenol	105-67-9	0.5133	0.5237	−0.0104
2,5-xylenol	95-87-4	0.5638	0.5163	0.0475
2,6-xylenol	576-26-1	0.4554	0.5027	−0.0473
3,4-xylenol	95-65-8	0.5763	0.5273	0.0490
3,5-xylenol	108-68-9	0.4852	0.5372	−0.0520
3-ethylphenol	620-17-7		0.4656	
2-ethylphenol	90-00-6	0.524	0.4864	0.0376
4-ethylphenol	123-07-9	0.524	0.5010	0.0230
diethyl ether	60-29-7	0.2811	0.3381	−0.0570
ethyl propyl ether	628-32-0	0.3462	0.3604	−0.0142

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Table 2. Continued

compounds	CAS	ω_{exp}	ω_{pred}	D^a
butyl methyl ether	628-28-4	0.3393	0.3463	−0.0070
tert-butyl methyl ether	1634-04-4	0.2661	0.2728	−0.0067
methyl pentyl ether	628-80-8	0.3470	0.3734	−0.0264
butyl ethyl ether	628-81-9	0.3854	0.3874	−0.0020
dipropyl ether	111-43-3	0.3701	0.3874	−0.0173
diisopropyl ether	108-20-3	0.3387	0.3483	−0.0096
dibutyl ether	6163-66-2	0.3459	0.4496	−0.1037
1,1-dimethylpropyl methyl ether	994-05-8	0.2975	0.2690	0.0285
1,1-dimethylpropyl ethyl ether			0.3253	
2-methoxyethanol	109-86-4	0.7311	0.7065	0.0246
2-propoxyethanol	2807-30-9	0.783	0.6597	0.1233
2-butoxyethanol	111-76-2	0.5213	0.6550	−0.1337
1-methoxy-2-propanol	107-98-2	0.7219	0.6714	0.0505
2-(2-methoxyethoxy)ethanol	111-77-3	0.8707	0.6661	0.2046
2-(2-ethoxyethoxy)ethanol	111-90-0	0.6808	0.6723	0.0085
2-(2-propoxyethoxy)ethanol			0.6736	
2-(2-butoxyethoxy)ethanol	112-34-5	0.6548	0.6816	−0.0268
1-propoxy-2-propanol	1569-01-3	0.8002	0.6557	0.1445
1-butoxy-2-propanol	5131-66-8	0.5008	0.6587	−0.1579
diphenyl ether	101-84-8	0.4717	0.4717	0.0000
methyl formiate			0.5060	
ethyl formiate			0.4656	
propyl formiate			0.4592	
butyl formiate			0.4683	
isobutyl formate	542-55-2	0.3896	0.4383	−0.0487
pentyl methanoate	638-49-3	0.5283	0.4862	0.0421
hexyl methanoate			0.5097	
heptyl methanoate			0.5367	
octyl methanoate	112-32-3	0.5871	0.5663	0.0208
methyl acetate	79-20-9	0.3313	0.2640	0.0673
ethyl acetate	141-78-6	0.3664	0.3151	0.0513
propyl acetate	109-60-4	0.3889	0.3715	0.0174
isopropyl acetate	108-21-4	0.3678	0.3578	0.0100
butyl acetate	123-86-4	0.4101	0.4236	−0.0135
isobutyl acetate	110-19-0	0.4340	0.3935	0.0405
pentyl acetate	628-63-7	0.4478	0.4727	−0.0249
hexyl acetate	142-92-7	0.5396	0.5199	0.0197
heptyl acetate	112-06-1	0.5953	0.5656	0.0297
octyl acetate	112-14-1	0.6514	0.6102	0.0412
nonyl acetate	143-13-5	0.7159	0.6539	0.0620
decyl acetate	112-17-4	0.7502	0.6970	0.0532
methyl propionate	554-12-1	0.3466	0.3809	−0.0343
ethyl propionate	105-37-3	0.3944	0.3999	−0.0055
propyl propionate	106-36-5	0.4487	0.4376	0.0111
butyl propionate	590-01-2	0.4754	0.4760	−0.0006
pentyl propionate	624-54-4		0.5148	
hexyl propionate	2445-76-3		0.5537	
heptyl propionate	2216-81-1		0.5928	
octyl propionate	142-60-9		0.6319	
methyl butanoate	623-42-7	0.3775	0.4156	−0.0381
ethyl butanoate	105-54-4	0.4011	0.4320	−0.0309
propyl butanoate	105-66-8	0.4484	0.4704	−0.0220
butyl butanoate	109-21-7	0.4852	0.5091	−0.0239
pentyl butyrate	540-18-1		0.5480	

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Table 2. Continued

compounds	CAS	ω_{exp}	ω_{pred}	D^a
hexyl butyrate	2639-63-6		0.5871	
heptyl butyrate	5870-93-9		0.6262	
octyl butyrate	110-39-4		0.6654	
2-methylpropyl butyrate	539-90-2	0.3949	0.4791	−0.0842
methyl isobutanoate	547-63-7	0.362	0.3853	−0.0233
ethyl isobutanoate	97-62-1	0.4264	0.4056	0.0208
propyl 3-methylbutanoate	557-00-6	0.4	0.5399	−0.1399
2-methylpropyl-3-methylbutanoate	589-59-3		0.5990	
3-methylbutyl butanoate	106-27-4		0.5180	
2-propenyl acetate	591-87-7	0.3879	0.3879	0.0000
2-ethenyl acetate			0.4177	
methyl pentanoate	624-24-8		0.4503	
ethyl pentanoate	539-82-2		0.4647	
propyl pentanoate	141-06-0		0.5034	
methyl caproate			0.4851	
ethyl caproate			0.4978	
propyl caproate	626-77-7		0.5367	
butyl caproate	626-82-4		0.5758	
pentyl caproate	540-07-8		0.6149	
hexyl caproate	6378-65-0		0.6541	
heptyl caproate			0.6933	
octyl caproate			0.7325	
methyl heptanoate	106-73-0		0.5197	
ethyl heptanoate	106-30-9		0.5310	
propyl heptanoate	7778-87-2		0.5701	
butyl heptanoate	5454-28-4		0.6092	
pentyl heptanoate	7493-82-5		0.6484	
hexyl heptanoate	1119-06-8		0.6876	
heptyl heptanoate	624-09-9		0.7269	
octyl heptanoate	5132-75-2		0.7661	
methyl caprylate	111-11-5		0.5542	
ethyl caprylate	106-32-1		0.5644	
propyl caprylate			0.6036	
buyyl caprylate			0.6428	
pentyl caprylate			0.6820	
hexyl caprylate	1117-55-1		0.7212	
heptyl caprylate	4265-97-8		0.7604	
octyl caprylate	2306-88-9		0.7997	
methyl pelargonate	1731-84-6		0.5943	
ethyl pelargonate	123-29-5		0.5979	
propyl pelargonate			0.6371	
butyl pelargonate			0.6763	
heptyl pelargonate			0.7904	
methyl caprate	110-42-9	0.6993	0.6230	0.0763
ethyl caprate	110-38-3		0.6314	
hexyl caprate			0.7884	
methyl undecanoate	1731-86-8		0.6629	
ethyl undecanoate	627-90-7		0.6650	
pentyl undecanoate	10484-11-4		0.7827	
methyl dodecanoate	111-82-0	0.6924	0.6914	0.0010
ethyl dodecanoate	106-33-2		0.6985	
butyl dodecanoate	106-18-3		0.7770	
methyl tridecanote			0.7255	
propyl tridecanote			0.7714	

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Table 2. Continued

compounds	CAS	ω_{exp}	ω_{pred}	D^a
methyl tetradecanote			0.7596	
ethyl tetradecanote			0.7657	
methyl pentadecanoate	7132-64-1		0.7936	
methyl palmitate	112-39-0		0.8275	
ethyl palmitate	628-97-7		0.8329	
propyl palmitate	2239-78-3		0.8721	
butyl palmitate	111-06-8		0.9114	
methyl margarate	1731-92-6		0.8614	
ethyl margarate			0.8664	
methyl stearate	112-61-8		0.8953	
ethyl stearate	111-61-5		0.9000	
propyl stearate	3634-92-2		0.9393	
butyl stearate	123-95-5	1.0246	0.9785	0.0461
methyl nonadecanoate	1731-94-8		0.9292	
ethyl nonadecanoate	18281-04-4		0.9336	
methyl eicosonoate			0.9630	
ethyl eicosonoate			0.9672	
methyl uneicosonate			0.9968	
methyl benenate			1.0306	
ebenenate			1.0343	
methyl tricosanoate	2433-97-8		1.0643	
ethyl tricosanoate	18281-07-7		1.0679	
methyl tetracosanoate	2442-49-1		1.0981	
dimethyl succinate	106-65-0	0.6223	0.6467	−0.0244
diethyl succinate	123-25-1	0.6649	0.6603	0.0046
dipropyl succinate	925-15-5		0.7307	
dibutyl succinate	141-03-7		0.8035	
dipentyl succinate			0.8778	
dimethyl glutarate	1119-40-0		0.6820	
diethyl glutarate	818-38-2		0.6951	
dipropyl glutarate			0.7669	
dimethyl adipate	627-93-0		0.7182	
diethyl adipate	141-28-6		0.7307	
dipropyl adipate	106-19-4		0.8035	
dibutyl adipate	105-99-7		0.8778	
dipentyl adipate			0.9531	
dihexyl adipate	110-33-8	1.0935	1.0290	0.0645
dioctyl adipate	103-23-1	1.0598	1.1821	−0.1223
dimethyl pimelate	1732-08-7		0.7550	
diethyl pimelate	2050-20-6		0.7669	
dipropyl pimelate			0.8405	
dibutyl pimelate			0.9153	
1-methylpropyl ethanoate	105-46-4	0.3954	0.4070	−0.0116
isobutyl acrylate	106-63-8	0.4573	0.4573	0.0000
methylamine	74-89-5	0.2814	0.2814	0.0000
dimethylamine	124-40-3	0.2999	0.2916	0.0083
ethylamine			0.2424	
propylamine	107-10-8	0.2798	0.3117	−0.0319
isopropylamine	75-31-0	0.2759	0.2545	0.0214
trimethylamine	75-50-3	0.2087	0.2050	0.0037
butylamine	109-73-9	0.3292	0.3694	−0.0402
isobutylamine	78-81-9	0.3627	0.3455	0.0172
sec-butylamine	13952-84-6	0.2815	0.3081	−0.0266
tert-butylamine	75-64-9	0.2748	0.2748	0.0000

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Table 2. Continued

compounds	CAS	ω_{exp}	ω_{pred}	D^a
diethylamine	109-89-7	0.3041	0.3359	−0.0318
pentylamine	110-58-7	0.4070	0.4212	−0.0142
cyclopentylamine	1003-03-8	0.3294	0.3294	0.0000
hexylamine	111-26-2	0.4577	0.4695	−0.0118
butyl ethylamine	13360-63-9		0.4543	
triethylamine	121-44-8	0.3162	0.3226	−0.0064
dipropylamine	142-84-7	0.4646	0.4503	0.0143
diisopropylamine	108-18-9	0.3883	0.3857	0.0026
cyclohexylamine	108-91-8	0.3604	0.3604	0.0000
dibutylamine	111-92-2	0.5600	0.5490	0.0110
1,2-ethanediamine	107-15-3	0.4789	0.4500	0.0289
1,3-propanediamine	109-76-2	0.50627	0.5034	0.0029
1,4-butanediamine	110-60-1		0.5520	
1,6-hexanediamine	124-09-4	0.6501	0.6422	0.0079
1,8-octanediamine	373-44-4		0.7277	
1,9-nonanediamine	646-24-2		0.7695	
1,10-decanediamine	646-25-3		0.8109	
1,12-dodecanediamine			0.8926	
benzenamine	62-53-3	0.4041	0.3824	0.0217
2-methylbenzenamine	95-53-4	0.3842	0.4211	−0.0369
3-methylbenzenamine	108-44-1	0.4348	0.4419	−0.0071
4-methylbenzenamine	106-49-0	0.4722	0.4529	0.0193
N-methylbenzenamine	100-61-8	0.4799	0.4799	0.0000
N-ethylbenzenamine	103-69-5		0.4594	
N,*N*-dimethylbenzenamine	121-69-7	0.4032	0.4171	−0.0139
N,*N*-diethylbenzenamine	91-66-7	0.4262	0.4093	0.0169
pyridine	110-86-1	0.2389	0.2535	−0.0146
2-methylpyridine	109-06-8	0.2990	0.2953	0.0037
3-methylpyridine	108-99-6	0.2978	0.2910	0.0068
4-methylpyridine	108-89-4	0.3021	0.2822	0.0199
2,3-dimethylpyridine	583-61-9	0.3123	0.3394	−0.0271
2,4-dimethylpyridine	108-47-4		0.3305	
2,5-dimethylpyridine	589-93-5	0.3596	0.3394	0.0202
2,6-dimethylpyridine	108-48-5	0.3453	0.3437	0.0016
3,4-dimethylpyridine	583-58-4	0.3063	0.3262	−0.0199
3,5-dimethylpyridine	591-22-0	0.3451	0.3351	0.0100
propanenitrile	107-12-0	0.3248	0.3059	0.0189
butanenitrile	109-74-0	0.3714	0.3673	0.0041
2-methylpropanenitrile	78-82-0	0.3384	0.3384	0.0000
pentanenitrile	110-59-8	0.4152	0.4225	−0.0073
3-methylbutanenitrile	625-28-5		0.3966	
2,2-dimethylpropanenitrile	630-18-2		0.1633	
hexanenitrile	628-73-9	0.4743	0.4734	0.0009
octanenitrile	124-12-9		0.5678	
decanenitrile	1975-78-6	0.6398	0.6564	−0.0166
chloroethane	75-00-3	0.1902	0.1826	0.0076
1-chloropropane	540-54-5	0.2277	0.2330	−0.0053
2-chloropropane	75-29-6	0.1986	0.2217	−0.0231
1-chlorobutane	109-69-3	0.2738	0.2810	−0.0072
2-chlorobutane	78-86-4	0.2907	0.2676	0.0231
2-chloro-2-methylpropane	507-20-0	0.1914	0.1914	0.0000
1-chloropentane	543-59-9	0.3328	0.3270	0.0058
2-chloropentane	625-29-6		0.3136	
1,1-dichloroethane	75-34-3	0.2339	0.2330	0.0009

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Table 2. Continued

compounds	CAS	ω_{exp}	ω_{pred}	D^a
bromoethane	74-96-4	0.2533	0.2530	0.0003
1-bromopropane	106-94-5	0.2848	0.2855	−0.0007
2-bromopropane	75-26-3	0.2432	0.2432	0.0000
1-bromobutane	109-65-9	0.3226	0.3221	0.0005
1-bromo-2-methylpropane	78-77-3		0.2962	
2-bromo-2-methylpropane	507-19-7		0.2312	
1-bromopentane	110-53-2		0.3605	
methylthioethane	624-89-5	0.2160	0.2238	−0.0078
1-methylthiopropane	3877-15-4	0.2737	0.2772	−0.0035
2-methylthiopropane	1551-21-9	0.2461	0.2519	−0.0058
1-methylthiobutane	628-29-5	0.3229	0.3268	−0.0039
2-methyl-2-methylthiopropane	6163-64-0	0.2334	0.2516	−0.0182
1-ethylthiopropane	4110-50-3		0.2803	
2-ethylthiopropane	5145-99-3		0.2550	
1-ethylthiobutane	638-46-0		0.3315	
2-ethylthio-2-methyl propane	14290-92-7	0.2861	0.2522	0.0339
1,2-dibromopropane	78-75-1		0.2766	
1,1,2-trichloroethane	79-00-5	0.2591	0.2600	−0.0009
methylthiomethane	75-18-3	0.1943	0.1747	0.0196
ethanethiol	75-08-1	0.1878	0.1643	0.0235
1-propanethiol	107-03-9	0.2353	0.2269	0.0084
2-propanethiol	75-33-2	0.2120	0.2017	0.0103
1-butanethiol	109-79-5	0.2714	0.2823	−0.0109
2-butanethiol	513-53-1	0.2506	0.2551	−0.0045
2-methyl-1-propanethiol	513-44-0	0.2522	0.2564	−0.0042
2-methyl-2-propanethiol	75-66-1	0.1914	0.2071	−0.0157
1-pentanethiol	110-66-7	0.3207	0.3334	−0.0127
1-hexanethiol	111-31-9	0.3676	0.3816	−0.0140
1-heptanethiol	1639-09-4	0.4193	0.4279	−0.0086
acetic acid	64-19-7	0.4665	0.6168	−0.1503
propanoic acid			0.6962	
acrylic acid	70-10-7	0.5180	0.5180	0.0000
butyric acid	107-92-6	0.6809	0.6811	−0.0002
2-methylpropanoic acid	79-31-2	0.6140	0.6441	−0.0301
pentanoic acid	109-52-4	0.6984	0.6844	0.0140
3-methylbutanoic acid	503-74-2	0.6480	0.6605	−0.0125
2-ethyl butyric acid	88-09-5	0.6326	0.6661	−0.0335
hexanoic acid	142-62-1	0.7380	0.6981	0.0399
heptanoic acid	111-14-8	0.7581	0.7183	0.0398
octanoic acid	124-07-2	0.7706	0.7429	0.0277
2-ethylhexanoic acid	149-57-5	0.8208	0.7160	0.1048
nonanoic acid	112-05-0	0.7724	0.7705	0.0019
decanoic acid	334-48-5	0.8060	0.8002	0.0058
isobutyl acid			0.6441	
3-methyl-pentanoic acid	105-43-1		0.6722	
4-methyl-pentanoic acid	646-07-1		0.6763	
2,2-dimethyl-butanoic acid	595-37-9	0.5671	0.5671	0.0000
2,3-dimethyl-butanoic acid			0.6443	
3,3-dimethyl-butanoic acid	1070-83-3		0.6428	
undecanoic acid	112-37-8	0.8427	0.8316	0.0111
lauric acid	143-07-7	0.8800	0.8641	0.0159
tridecanoic acid	638-53-9	1.0042	0.8977	0.1065
tetradecanoic acid	544-63-8	0.9356	0.9320	0.0036
pentadecanoic acid	1002-84-2	0.9586	0.9670	−0.0084

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Table 2. Continued

compounds	CAS	ω_{exp}	ω_{pred}	D^a
palmitic acid	57-10-3	1.0611	1.0024	0.0587
argaric caid			1.0383	
stearic acid	57-11-4	1.0360	1.0745	−0.0385
nonadecanoic acid	646-30-0	1.0628	1.1111	−0.0483
succinic acid	110-15-6	0.9922	1.0628	−0.0706
methylsuccinic acid	498-21-5		1.0384	
glutaric acid	110-94-1	0.9590	1.0451	−0.0861
ethylsuccinic acid	636-48-6		1.0120	
2,2-dimethylsuccinic acid	597-43-3		0.9143	
adipic acid	124-04-9	1.0506	1.0409	0.0097
heptanedioic acid	111-16-0	1.1158	1.0460	0.0698
octanedioic acid	505-48-6	1.1471	1.0578	0.0893
nonanedioic acid	123-99-9	1.1720	1.0745	0.0975
sebacic acid	111-20-6	1.2053	1.0948	0.1105
undecanedioic acid	1852-04-6		1.1181	
dodecanedioic acid	693-23-2		1.1436	
tridecanedioic acid	505-52-2		1.1709	
tetradecanedioic acid	821-38-5		1.1997	
hexadecanedioic acid	505-54-4		1.2298	
3-methyl glutaric acid	626-51-7		1.0151	
2,2-diethylsuccinic acid	5692-97-7		0.9227	
trimethylglutaric acid			0.9861	
tetramethylsuccinic acid	630-51-3		0.8175	
triethylsuccinic acid	2103-18-6		0.9177	
tetraethylsuccinic acid	4111-60-8		0.8368	
benzoic acid	65-85-0	0.6039	0.6294	−0.0255
2-methylbenzoic acid	118-90-1	0.6572	0.6307	0.0265
3-methylbenzoic acid	99-04-7		0.6479	
4-methylbenzoic acid	99-94-5	0.6610	0.6589	0.0021
2-ethylbenzoic acid	612-19-1		0.6162	
3-ethylbenzoic acid	619-20-5		0.6334	
4-ethylbenzoic acid	619-64-7		0.6444	
2,3-dimethylbenzoic acid	603-79-2		0.6337	
2,4-dimethylbenzoic acid	611-01-8		0.6619	
2,5-dimethylbenzoic acid	610-72-0		0.6681	
2,6-dimethylbenzoic acid	632-46-2		0.6337	
3,4-dimethylbenzoic acid	619-04-5		0.6619	
3,5-dimethylbenzoic acid	499-06-9		0.6681	
2,3,4-trimethylbenzoic acid	1076-47-7		0.6461	
2,3,5-trimethylbenzoic acid	2437-66-3		0.6633	
2,3,6-trimethylbenzoic acid	2529-36-4		0.6461	
2,4,5-trimethylbenzoic acid	528-90-5		0.6743	
2,4,6-trimethylbenzoic acid	480-63-7		0.6633	

[a] $D = \omega_{exp} - \omega_{pred}$.

center of the group in the molecular formula, N_j for the number of each group that the noncarbon element forms in the center, N for the total number of groups, P_k for the position correlation factor, and M is molecular weight. The hyperbolic tangent function is used especially for the groups whose center is not a saturated carbon atom. For instance, if there is the Cb−(C), Cd−Cd, or Cb−(H) group in some organic compounds, the hyperbolic tangent function should be considered. The chemical groups found and used in this study are extensively presented in Table 1. The values computed for the group contributions and the position factor contributions are also listed in Table 1. In addition, our method developed is applicable only to comparatively low molar mass compounds involving carbon chain from C2 to C18.

COMPARISON METHOD

Constantinou and Gani[12] proposed their second-order GC method to the estimation of the acentric factor for a variety of

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organic compounds (shown as eq 4).

$$w = 0.4085\{\ln[\sum_k N_k(w_1k) + W\sum_j M_j(w_2j) + 1.1507]\}^{(1/0.5050)} \quad (4)$$

where w_1k is the contribution of the first-order group type k, which occurs N_k times, and w_2j is the contribution of the second-order group type j, with M_j occurrences in a compound. The constant W is used to distinguish the second-level estimation (where both first- and second-order group contributions are involved, so $W = 1$) from the first-level estimation (only a first-order approximation, so $W = 0$).

RESULTS AND DISCUSSION

A. Prediction of the Acentric Factor. The results of the reference compounds obtained using the new positional distributive contribution method are presented in Table 2. Also, to illustrate the application of the proposed method, a detailed procedure for ω estimation is given in Appendix A. In fact, during our investigation, about 907 organic compounds were considered, and nearly 430 organic compounds without ω experimental data. Results listed in Table 2 show that, for about 477 organic compounds with ω experimental data, the predicted ω agrees well with the "experimental results", which indicates that our new positional distributive contribution method for predicting ω has good overall accuracy. In addition, for those 430 organic compounds without ω experimental data, the predicted ω is also given and listed in Table 2.

Table 3 compares ω predictions obtained using our method and the method of Constantinou and Gani (CG method). Also, the overall average absolute difference (AAD) between experimental and predicted values for each group of molecules as well as the overall mean differences δ and the average mean differences $\overline{\delta}$ are summarized in Table 3. Results listed in Tables 3 show that, with our method, satisfactory prediction results could be obtained; the AAD for ω prediction of 477 organic compounds is 0.0252, and $\overline{\delta}$ is 5.72 %. Moreover, the average estimation errors did not exceed 11 % for all of the chemical families under study.

$$D = \omega_{exp} - \omega_{pred} \quad (5)$$

$$AAD = \frac{\sum|\omega_{exp} - \omega_{pred}|}{n} \quad (6)$$

$$\delta = \left|\frac{\omega_{exp} - \omega_{pred}}{\omega_{exp}}\right| \quad (7)$$

$$\overline{\delta} = \frac{1}{N}\sum_n \left|\frac{\omega_{exp} - \omega_{pred}}{\omega_{exp}}\right| \quad (8)$$

In the case of the Constantinou and Gani method, the AAD is 0.0569, and $\overline{\delta}$ is 14.58 % for the ω prediction of 477 organic compounds. It is true that for about 125 alkanes and cycloalkanes, good correlation results could be obtained with Constantinou and Gani method, where the AAD is 0.0206 and $\overline{\delta}$ is 4.78 %. However, it is noteworthy that the Constantinou and Gani method failed to correlate ω data of amines and pyridines and nitriles and alkane thiols, with overall average absolute percentage deviations of 32.41 % and 61.46 %, respectively. While, with our position distribution contribution method, the overall average absolute percentage deviation is 4.07 % and 4.02 %, respectively, for amines and pyridines, and nitriles and alkane thiols.

Table 3. Comparison of ω Predicted with Constantinou and Gani Method and Our Method for Various Class Organic Compounds[a]

		Constantinou and Gani method		this work	
chemical family	samples	AAD	100 $\overline{\delta}$	AAD	100 $\overline{\delta}$
alkanes and cycloalkanes	125	0.0206	4.78	0.0130	4.08
alkenes	61	0.0269	11.49	0.0137	5.03
aromatics	44	0.0242	6.86	0.0156	4.13
ketones and aldehydes	37	0.0431	11.07	0.0345	8.52
alcohols	48	0.1102	19.15	0.0613	10.39
acids	32	0.0489	6.35	0.0418	5.01
esters and ether oxides	57	0.0820	16.24	0.0434	8.39
bromo chloroalkanes	12	0.0481	18.72	0.0062	2.60
amines and pyridines	37	0.1027	32.41	0.0141	4.07
nitriles and alkane thiols	24	0.1826	61.46	0.0106	4.02
overall	477	0.0569	14.58	0.0252	5.72

[a] AAD is the overall average absolute difference, and $\overline{\delta}$ is the average mean differences.

Therefore, it could be demonstrated that the proposed method is more precise and stable than the Constantinou and Gani method for ω prediction. Further, our method appears to be as accurate as the experimental data used to establish the group contributions and has a wide range of applicability. As a consequence, our new simple model could give lower deviations and can be used with confidence in thermodynamic and engineering calculations.

B. Uncertainty of This New Method. According to the F distribution function, the degree of confidence is calculated with the incomplete β function which could be calculated from the λ function. The results show that the correlation coefficient is 0.9833, the F distribution value is 107.1, and the degree of confidence is 0.99, which further confirms a greater precision of our positional distributive contribution method for the prediction of ω.

CONCLUSION

In this work, the positional distributive contribution method is extended for the prediction of the acentric factor ω of a variety of pure organic compounds. Contributions for compounds containing carbon, hydrogen, oxygen, nitrogen, chlorine, and sulfur were reported, and a position distribution function has been developed which could distinguish between the thermodynamic properties of all isomers of organic compounds including *cis*- and *trans*- or *Z*- and *E*-structures. The prediction results indicate that our model provides very satisfactory results. The overall average absolute difference and the relative derivation for ω predictions of 477 organic compounds are found to be 0.0252 and 5.72 %, respectively. Comparing results demonstrated that our method performed well both in accuracy and in stability. More importantly, the higher prediction accuracy of the proposed method shown in our previous works and this work suggests that it is possible to use a similar framework to predict various properties of organic compounds containing various functional groups, which further demonstrated the universality of our proposed method.

APPENDIX A

Example 1. Prediction of ω for ethyl isobutanoate.

This compound is decomposed in position groups as follows: 1 C−$(CH_2)(H)_3$; 2 C−$(CH)(H)_3$; 1 C−$(C)_2(CO)(H)$; 1 C−$(C)(O)(H)_2$; 1 CO−$(CH)(O)$; 1 O−$(CO)(CH_2)$. The total number of groups is $N = 7$.

According to the IUPAC nominating method, since the position of the CO−(CH)(O) group is 3, then the position correlation factor P for the CO−(CH)(O) group is 3. The molecular weight is $M = 116.16$.

The CO−(CH)(O) group and the O−$(CO)(CH_2)$ group are the groups whose center is not a saturated carbon atom; therefore, N_j is 1 and 1, respectively.

From the contributions in Table 1, ω is estimated by eq 2:

$$\omega = 7.86948 - 0.02842 - 2\cdot 0.026407 + 0.24527 + 0.010102 - 0.111642\tanh(1/7) + 0.37326\tanh(1/7) - 3\cdot 0.0056631 - 7.62053\exp(1/116.16) + 0.025051\exp(1/7) = 0.4056$$

Therefore, the calculated ω result is 0.4056 while the experimental ω is 0.4264.

Example 2. Prediction of ω for ethylbenzene.

This compound is decomposed in position groups as follows: 5 Cb−(H); 1 Cb−(C); 1 C−$(Cb)(H)_2(C)$; 1 C−$(H)_3(CH_2)$.

The five Cb−(H) groups and the one Cb−(C) group are the groups whose center is not a saturated carbon atom; therefore, N_j is 5 and 1, respectively. The total number of groups is $N = 8$. The molecular weight is $M = 106.17$.

From the contributions in Table 1, ω is estimated by eq 2:

$$\omega = 7.86948 + 0.13514 - 0.028420 + 0.0052792\tanh(5/8) - 0.201254\tanh(1/8) - 7.62053\exp(1/106.17) + 0.025051\exp(1/8) = 0.2898$$

Therefore, the calculated ω result is 0.2898, while the experimental ω is 0.3035.

Example 3. Estimation of ω of 2,3-dimethylpyridine.

This compound is decomposed in position groups as follows: 3 Cb−(H); 2 Cb−(C); 2 C−$(Cb)(H)_3$; 1 NI−$(Cb)_2$. The total number of groups is $N = 8$. The molecular weight is $M = 107.16$.

The three Cb−(H) groups, two Cb−(C) groups, and one NI-$(Cb)_2$ group are the groups whose center is not a saturated carbon atom; therefore, N_j is 3, 2, and 1, respectively.

Also, the corrections for pyridines, C_{ob} and C_{mb}, take into account alkyl ligands in position ortho and meta with respect to the N element, respectively.

From the contributions in Table 1, ω is estimated by eq 2:

$$\omega = 7.86948 + 2\cdot 0.09178058 + \tanh(3/8)\cdot 0.005279216 - \tanh(2/8)\cdot 0.020125448 + \tanh(1/8)\cdot 0.413905275 - 0.024913528 - 0.029219287 - 7.62053\exp(1/107.16) + 0.025051\exp(1/8) = 0.3394$$

Therefore, the calculated ω result is 0.3394, while the experimental ω is 0.3123.

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