J Mol Model (2008) 14:109–134
DOI 10.1007/s00894-007-0256-x

ORIGINAL PAPER

Topological research on diamagnetic susceptibilities of organic compounds

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Received: 28 August 2007 / Accepted: 14 November 2007 / Published online: 3 January 2008

Abstract A novel molecular connectivity index, ${}^{m}\chi'$, based on the adjacency matrix of molecular graphs and novel atomic valence connectivities, δ_i', for predicting the molar diamagnetic susceptibilities of organic compounds is proposed. The δ_i' is defined as: $\delta_i' = \delta_i^v \cdot E_i/12.625$, where δ_i^v and E_i are the atomic valence connectivity and the valence orbital energy of atom i, respectively. A good QSPR model for molar diamagnetic susceptibilities can be constructed from ${}^{0}\chi', {}^{1}\chi', {}^{2}\chi'$ and ${}^{4}\chi_p'$ using multivariate linear regression (MLR). The correlation coefficient r, standard error, and average absolute deviation of the MLR model are 0.9918, 5.56 cgs, and 4.26 cgs, respectively, for the 721 organic compounds tested (training set). Cross-validation using the leave-one-out method demonstrates that the MLR model is highly reliable statistically. Using the MLR model, the average absolute deviations of the predicted values of molar diamagnetic susceptibility of another 360 organic compounds (test set) is 4.34 cgs. The results show that the current method is more effective than literature methods for estimating the molar diamagnetic susceptibility of an organic compound. The MLR method thus provides an acceptable model for the prediction of molar diamagnetic susceptibilities of organic compounds.

Keywords Diamagnetic susceptibility · Organic compound · Connectivity index

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Introduction

The diamagnetic susceptibility, χ, of a compound is an important physicochemical property. When a material is placed in a magnetic field $\boldsymbol{H}$, a magnetization (magnetic moment per unit volume) $\boldsymbol{M}$, which is related to $\boldsymbol{H}$ by $\boldsymbol{M}=\kappa\boldsymbol{H}$ [1–4], where κ is called the volume susceptibility, is induced in the material. Since $\boldsymbol{H}$ and $\boldsymbol{M}$ have the same dimensions, κ is dimensionless. A more useful parameter is the molar susceptibility, χ_m, defined by

$$\chi_m = \kappa V_m = \kappa M/\rho \tag{1}$$

where V_m is the molar volume of the substance, M the molar mass, and ρ the mass density. Using the cgs system, the customary units for χ_m are $cm^3 \cdot mol^{-1}$, with the corresponding SI units being $m^3 \cdot mol^{-1}$.

Substances that have no unpaired electron orbital or spin angular momentum generally have negative values of χ_m and are called diamagnetic. Their molar susceptibility varies only slightly with temperature. Substances with unpaired electrons, which are termed paramagnetic, have positive χ_m and show much stronger temperature dependence, varying roughly as $1/T$. The net susceptibility of a paramagnetic substance is the sum of the paramagnetic and diamagnetic contributions, but the former almost always dominates. A substance for which $\chi_m<0$ is diamagnetic, and its molar diamagnetic susceptibility can be obtained from the Langevin-Pauli formula [1–4].

The theoretical and practical importance of this property has long interested chemists as it could be exploited for the determination and prediction of the diamagnetic susceptibility of compounds [4]. For many years, experimental and theoretical efforts in the field of diamagnetic susceptibilities of compounds have been devoted to the determination of this property for complex systems in different ways [5–10].

Interest in theoretical treatments for magnetic susceptibility dates from the beginning of the twentieth century. Magnetic susceptibilities of stable organic species have long been observed to be approximately fit by a sum of atomic contribution, the so-called Pascal's constants [3, 4], which have been used successfully in the prediction of diamagnetic susceptibilities of organic compounds, and are still in use even today [4]. A subsequent expansion, motivated by the simple quantum chemical treatment, was developed by Hameka [11–15] to describe the diamagnetic susceptibilities of several classes of organic compounds. Hameka's approach considers not only atomic contributions, but also the contributions of bonds and bond–bond interactions. However, a large number of experimental values of diamagnetic susceptibilities are needed in order to obtain that large family of parameters. Although theoretical calculation of diamagnetic susceptibility can be attractive in some simple cases, most results thus obtained are quantitatively incomparable with experimental values [16]. Subsequent studies included quantum chemical approaches such as the path-integral formulation of quantum mechanics, Weizsäcker energy of many-electron systems, or density-functional methods [17–20], integrated molecular transforms [21], and graph theoretical concepts [22–27].

The diamagnetic property of a compound is determined mainly by its molecular structure rather than by its bulk as a whole [28]. Hence, the application of graph theory in this context may have some merit, although the structure here is represented approximately by the graph without taking into account geometrical details. In fact, many attempts have been made in this direction, ranging from the Wiener [29] or Randic index [30] for alkanes, and the more sophisticated connectivity indices of Kier and Hall [22, 31] for both alkanes and aliphatic alcohols, to the cluster expansion method [22, 32]. It is apparent that a tendency in the construction of new topological indices was followed [33] as more electronic structure information was incorporated into the graph to obtain a so-called chromograph, thus allowing elements other than C, N, O, F, C1, etc. to be fully described; the method can be largely extended for use with inorganic or organometallic compounds [24, 34–40].

In recent years, Qing [41], Feng [42], and Mu [43, 44], among others, have developed several QSPR/QSAR models to estimate the diamagnetic susceptibilities of inorganic compounds by using various model parameters. The present study defines a novel atomic valence connectivity index, δ_i', based on the valence orbital energy of atom i, the number of electrons of atom i, the number of valence electrons of atom i and the number of hydrogens connected with atom i. A new novel molecular connectivity index based on the Kier-Hall [22] index and δ_i' is proposed. The novel molecular connectivity index correlates well with the diamagnetic susceptibilities of organic compounds.

Molecular descriptors

Molecular connectivity indexes, which contain a large amount of information about the molecule, including the numbers of hydrogen and non-hydrogen atoms bonded to each nonhydrogen atom, the details of the electronic structure of each atom, and the molecular structural features (paths, branches, clusters and rings), have been widely used as structure descriptors [22]. The details of their definition and calculation methods can be found elsewhere [22]. The general expression for the mth-order molecular connectivity index is defined as follows [22]:

$$ {}^{m}\chi_k = \sum_{j=1}^{n_m} \left(\prod_{i=1}^{m+1} \delta_i \right)_j^{-1/2} \tag{1} $$

where m is the order of the molecular connectivity index, k denotes a contiguous path type of fragment, which is divided into paths (P), clusters(C), path/clusters(PC) and chains (cycles)(CH), n_m is the number of the relevant paths, and δ_i is the simple atomic connectivity index, equal to the numbers of non-hydrogen atoms to which the ith non-hydrogen atom is bonded. The δ_i is defined as:

$$ \delta_i = \left(Z_i^v - h_i \right) \tag{2} $$

where Z_i^v is the number of valence electrons, and h_i the number of hydrogens connected with atom i. If δ_i is replaced by δ_i^v, the atomic valence connectivity index, we can obtain the expression for the mth-order molecular valence connectivity index, ${}^{m}\chi_k^v$, as follows:

$$ {}^{m}\chi_k^v = \sum_{j=1}^{n_m} \left(\prod_{i=1}^{m+1} \delta_i^v \right)_j^{-1/2} \tag{3} $$

The δ_i^v is defined as:

$$ \delta_i^v = \frac{\left(Z_i^v - h_i \right)}{\left(Z_i - Z_i^v - 1 \right)} \tag{4} $$

where Z_i is the number of electrons of atom i, Z_i^v the number of valence electrons, and h_i the number of hydrogens connected with atom i.

In our study, we found that the δ_i^v value can be used not only to distinguish different atoms, but also to reflect some atomic characteristics. However, the δ_i^v value does not distinguish the precise chemical environment of an atom. For instance, the δ_i^v value of the carbon atom is 3 in all the following atom groups: "sssCH", "dsCH", and "tCH" ("s" for single bond, "d" for double, "t" for triple). Therefore, we defined a novel δ_i' for all atoms using a united formula

according to the structural characteristics of different atoms. The $\delta_i^{'}$ value is defined as:

$$\delta_i' = \delta_i^v \cdot \frac{E_i}{E_{C-sp^3}} = \frac{\left(Z_i^v - h_i\right)}{\left(Z_i - Z_i^v - 1\right)} .E_i/12.625 \quad (5)$$

where Z_i is the number of electrons of atom i, Z_i^v the number of valence electrons, h_i the number of hydrogens connected with atom i, E_i the valence orbital energy, and the constant12.625 is the sp^3 hybrid orbital energy of the carbon atom.

For the hybrid orbital (sp^n) composed of the s and p orbitals, E_i is defined as [45]:

$$E_i = \left(E_s + n.E_p\right)/(n+1) \quad (6)$$

For saturated hydrocarbon, $E_i = E_{C-sp^3} = 12.625$, $\delta_i' = \delta_i^v$. The E_i and $\delta_i^{'}$ value for some atoms in different atom groups are calculated from Eqs. 5 and 6, and are listed in Table 1.

When we use the delta value $\delta_i^{'}$ instead of the original delta value δ_i^v of molecular connectivity index, a novel set of valence molecular connectivity indexes is obtained. The novel connectivity index ${}^m\chi'$ can be defined as follows:

$${}^m\chi_k' = \sum_{j=1}^{n_m} \left(\prod_{i=1}^{m+1} \delta_i^{'} \right)_j^{-1/2} \quad (7)$$

where m is the order of the molecular connectivity index. We calculated the ${}^0\chi'$, ${}^1\chi'$, ${}^2\chi'$, ${}^3\chi_p^{'}$, ${}^3\chi_c^{'}$, ${}^4\chi_p^{'}$, ${}^4\chi_c^{'}$ ${}^5\chi_p^{'}$, ${}^4\chi_{pc}^{'}$, and ${}^5\chi_{\mathrm{pc}}^{'}$ of 1,081 organic compounds.

Data set

The quantitative structure–property relationships (QSPR) treatment begins with assembly of the dataset. Experimental molar diamagnetic susceptibilities (χ_{m}) data were compiled from references [27, 46–48], and [49]. A total of 1,081 organic compounds with extensive structural diversity were selected as the dataset (Tables 2, 3). The quality and robustness of the predictive power of a QSPR model depends heavily on the diversity of the dataset. To select significant descriptors for the QSPR model that capture all the underlying interaction mechanisms, it is advisable to represent as many structural features as possible in the dataset. The working dataset included hydrocarbons (alkanes, cycloalkanes, alkenes, cycloalkenes, alkynes), non-hydrocarbons (carboxylic acids, alcohols, aldehydes, ketones, amines, halides, ethers, esters, acid halides, amides, nitro compounds, nitriles, nitrates, sulfides, thiocyanates) and their substituted compounds.

Multi-linear regression models

Linear QSPR models can be developed using several statistical techniques, such as multivariate linear regression,

Table 1 Atomic attributes and $\delta_i^{'}$ values for organic compounds

No	Atom group[a]	δ_i^v	E_i	$\delta_i^{'}$	No	Atom group	δ_i^v	E_i	$\delta_i^{'}$
1	sCH3	1	12.625	1.0000	19	tN	5	17.400	6.8911
2	ssCH2	2	12.625	2.0000	20	dN	5	16.433	6.5081
3	sssCH	3	12.625	3.0000	21	ddN	5	17.400	6.8911
4	ssssC	4	12.625	4.0000	22	ddsN	20[c]	16.433	26.0325
5	dCH2	2	13.067	2.0700	23	dssN	10[b]	16.433	13.0163
6	dsCH	3	13.067	3.1050	24	sSH	0.56	10.400	0.4576
7	dssC	4	13.067	4.1400	25	ssS	0.67	10.400	0.5492
8	ddC	4	13.950	4.4198	26	dS	0.67	13.667	0.7217
9	tCH	3	13.950	3.3149	27	dssS	1.33[b]	13.667	1.4434
10	stC	4	13.950	4.4198	28	ddssS	2.67[c]	12.850	2.7142
11	sOH	5	13.600	5.3861	29	sPH2	0.33	10.500	0.2772
12	ssO	6	13.600	6.4634	30	ssPH	0.44	10.500	0.3696
13	dO	6	18.567	8.8239	31	sssP	0.56	10.500	0.4620
14	sNH2	3	14.500	3.4445	32	dsssP	2.22[c]	10.500	1.8482
15	ssNH	4	14.500	4.5941	33	sF	7	17.400	9.6475
16	sssN	5	14.500	5.7426	34	sCl	0.78	13.000	0.8009
17	dNH	4	16.433	5.2065	35	sBr	0.26	11.900	0.2444
18	dsN	5	16.433	6.0581	36	sI	0.16	10.500	0.1294

[a] Symbols: *s* single bond, *d* double, *t* triple
[b] $\delta_i^v = 2\left[\left(Z_i^V - h_i\right)/\left(Z_i - Z_i^v - 1\right)\right]$
[c] $\delta_i^v = 4\left[\left(Z_i^v - h_i\right)/\left(Z_i - Z_i^v - 1\right)\right]$

Table 2 Experimental and calculated diamagnetic susceptibilities of 721 organic compounds (training set). Compounds with standard deviations larger than two standard errors are in bold

No	Compounds	$-\chi_M(10^{-6}$cgs)		
		Experimental	Calculated 1	Calculated 2
1	Acetylene	12.50	16.31	15.60
2	Fluoromethane	17.80	18.76	17.84
3	ethylene	18.80	20.80	19.50
4	formic acid	19.90	19.74	19.61
5	methyl alcohol	21.40	20.78	19.16
6	cyanogen	21.60	13.82	13.75
7	acetaldehyde	22.70	28.11	27.55
8	cyanamide	24.80	20.36	20.54
9	dimethyl ether	26.30	33.10	30.92
10	methylamine	27.00	22.78	21.64
11	acetonitrile	28.00	26.79	26.23
12	ethylene oxide	30.50	29.12	29.40
13	propene	31.50	33.22	31.87
14	acetic acid	31.54	32.34	31.81
15	1,3-butadiene	32.10	37.08	35.95
16	trifluoroethene	32.20	29.35	30.16
17	urea	33.50	27.44	27.85
18	ethyl alcohol	33.60	32.47	31.26
19	acetamide	34.10	33.80	33.58
20	propionaldehyde	34.32	39.42	39.22
21	nitroethane	35.40	37.82	42.33
22	1,2-butadiene	35.60	39.72	38.42
23	chloroethylene	35.90	34.92	33.78
24	allyl alcohol	36.70	35.71	34.75
25	triazine	37.90	43.00	44.85
26	thioacetic acid	38.40	43.66	42.91
27	chlorodifluoromethane	38.60	34.36	34.52
28	acetyl chloride	38.90	41.62	41.16
29	oxamide	39.00	38.95	40.13
30	glycine	39.60	36.73	37.00
31	cyclobutane	40.00	46.41	47.90
32	1-amine-2-propene	40.10	37.40	36.82
33	pyridazine	40.50	46.12	47.39
34	1-butene	41.00	44.60	43.53
35	difluoroethanol	41.30	36.64	36.58
36	carbon disulfide	42.20	40.01	39.76
37	thioacetamide	42.45	45.06	44.71
38	methyloxirane	42.50	40.99	41.22
39	cis-2-butene	42.60	45.95	44.38
40	methyl bromide	42.80	50.27	48.00
41	tetranitromethane	43.00	54.79	75.07
42	ethyl formate	43.00	44.38	43.68
43	furan	43.09	40.94	40.82
44	pyrimidine	43.10	45.89	47.20
45	trifluoroacetic acid	43.30	38.83	40.40
46	propionic acid	43.50	43.97	43.70
47	sulfamide	44.40	34.68	36.85
48	acetoxime	44.42	34.59	33.88
49	n-methyl urea	44.60	40.27	40.28
50	dimethyl sulfide	**44.90**	**57.61**	**55.89**
51	n-propyl alcohol	45.18	43.36	42.53
52	chlorotrifluoromethane	45.30	36.80	37.43
53	methyl ethyl ketone	45.50	51.76	51.22
54	ethyl-iso-cyanate	45.60	42.89	43.21

Table 2 (continued)

No	Compounds	$-\chi_M(10^{-6}cgs)$		
		Experimental	Calculated 1	Calculated 2
55	isopropyl alcohol	45.79	43.69	42.68
56	2-methyl-1,3-butadiene	46.00	49.13	47.83
57	malonic acid	46.30	46.71	47.35
58	iso-butyraldehyde	46.38	50.45	50.46
59	1,2-ethanediamine	46.50	37.88	37.87
60	dichloromethane	46.60	44.71	44.33
61	furfural	47.20	52.49	53.02
62	dimethoxymethane	47.30	48.80	46.17
63	succinic anhydride	47.50	52.95	54.36
64	1-chloro-2-propene	47.80	46.43	45.63
65	ethyl vinyl ether	47.90	49.71	47.96
66	carbonyl chloride	47.90	43.20	42.96
67	chloroacetic acid	48.10	45.81	45.80
68	methylol urea	48.30	43.07	43.42
69	1,3-cyclohexadiene	48.60	58.16	58.34
70	pyrrole	48.60	41.80	42.75
71	pyridine	48.70	49.25	49.94
72	fluorodichloromethane	48.80	45.51	45.51
73	2,3-pentadiene	49.10	52.78	51.02
74	chlorotrifluoroethylene	49.10	43.55	44.13
75	1,1-dichloroethylene	49.20	47.86	47.09
76	butyronitrile	49.40	49.43	49.40
77	maleic acid	49.60	52.60	53.13
78	thioglycollic acid	50.00	51.46	49.04
79	*2-butyne-1,4-diol*	50.30	47.50	46.71
80	alanine	50.50	48.70	48.87
81	thiophosgene	50.60	54.12	54.18
82	chloroacetone	50.90	53.60	53.31
83	cis-1,2-dichloroethylene	51.00	49.37	48.19
84	cyclopentanone	51.63	58.61	59.59
85	1,4-dioxane	52.16	56.26	55.85
86	dichlorodifluoromethane	52.20	47.40	47.78
87	acetic anhydride	52.80	57.21	56.51
88	iso-amylene	53.70	55.66	54.76
89	barbituric acid	53.80	61.19	63.93
90	cyclooctatetraene	**53.90**	**69.31**	**69.28**
91	ethyl acetate	54.10	57.24	55.88
92	2-butene-1,4-diol(cis)	54.30	51.08	50.14
93	1-pentene	54.60	55.81	54.77
94	1,2-epoxybutane	54.80	52.75	52.82
95	pyrrolidine	54.80	53.36	54.04
96	acetoxime-o-methyl-ether	54.87	47.52	45.79
97	2,4-pentanedione	54.90	62.59	62.35
98	methyl propionate	55.00	56.90	55.59
99	*propyl formate*	55.00	55.39	54.94
100	n-butyric acid	55.10	55.14	54.94
101	diethyl ether	55.10	57.24	55.26
102	N,N-dimethyl urea	55.10	52.15	52.00
103	N-ethyl urea	55.50	52.12	52.17
104	dimethyl oxalate	55.70	61.65	60.39
105	cytosine	55.80	56.33	58.67
106	1-chloropropane	56.00	53.99	53.43
107	2-aminothiazole	56.00	58.25	61.00
108	iso-butyraldoxime	56.10	57.11	56.77

Table 2 (continued)

No	Compounds	$-\chi_M(10^{-6}cgs)$		
		Experimental	Calculated 1	Calculated 2
109	N,N'-dimethyl urea	56.30	53.24	52.70
110	allyl acetate	56.70	60.43	59.38
111	diethylamine	56.80	58.74	57.49
112	ethyl carbamate	57.00	50.74	50.17
113	thymidine	57.10	66.81	69.45
114	glycerol	57.10	48.94	48.36
115	2,3-dimethyl-1,3-butadiene	57.20	61.32	59.76
116	iodomethane	57.20	64.30	58.26
117	methyl methacrylate	57.30	61.62	60.06
118	thiophene	57.30	56.02	57.96
119	butane	57.40	52.17	51.33
120	1,1-dichloroethane	57.40	54.65	54.67
121	tert-butyl alcohol	57.42	54.43	53.71
122	cyclohexene	57.50	63.89	64.20
123	pentanal	57.50	61.68	61.70
124	sec-butyl alcohol	57.68	55.19	54.29
125	methylmaleic acid	57.84	65.05	65.14
126	succinic acid	58.00	57.83	58.58
127	diethyl ketone	58.10	63.78	63.06
128	propylenediamine	58.10	49.48	49.48
129	dichloroacetic acid	58.20	58.43	58.89
130	fluorobenzene	58.40	55.64	56.18
131	propane-1-thiol	58.50	59.59	56.68
132	1-methylpyrrole	58.56	54.06	54.60
133	trichlorofluoromethane	58.70	57.61	58.24
134	n-butylamine	58.90	56.26	55.82
135	nitrosobenzene	59.10	61.13	62.37
136	cyclopentane	59.18	58.65	59.03
137	N-nitrosodiethylamine	59.30	67.40	67.27
138	fluorobromoacetic acid	59.50	60.45	59.85
139	2-methylthiazole	59.56	64.59	66.77
140	methyl acetoacetate	59.60	67.44	66.75
141	dimethyl isoxazole	59.70	62.78	62.39
142	isobutylamine	59.80	55.87	55.66
143	3-methylpyridine	59.80	61.65	61.89
144	1,3,5-cycloheptatriene	59.80	63.66	63.71
145	2-methylpyrrole	60.10	54.36	54.76
146	phenol	60.21	57.15	57.12
147	benzaldehyde	60.78	64.05	64.75
148	2,3-hexadiene	60.90	64.21	62.68
149	perfluoropropionic acid	61.00	54.81	57.41
150	*tropolone*	61.00	68.78	69.39
151	1,4-cycloheptadiene	61.00	69.22	69.37
152	cyanuric acid	61.50	56.91	58.43
153	1,3-butanediol	61.80	57.55	56.73
154	nitrobenzene	61.80	62.93	68.15
155	cyclohexanone	62.00	69.82	70.82
156	butyryl chloride	62.10	64.78	64.23
157	r-aminobutyric acid	62.10	59.01	59.46
158	acetonylacetone	62.51	73.61	73.59
159	n-butyl cyanide	62.80	60.59	60.63
160	aniline	62.95	58.65	58.89
161	2,2-dimethylpropane	63.10	61.59	61.41
162	dimethyl oxamide	63.20	63.91	64.25

Table 2 (continued)

No	Compounds	$-\chi_M(10^{-6}cgs)$		
		Experimental	Calculated 1	Calculated 2
163	nitrosopiperidine	63.40	73.29	75.05
164	iso-butyryl chloride	63.90	64.60	64.33
165	cyclopentanol	64.00	62.10	62.39
166	cyclohexenol	64.10	68.35	68.53
167	N,N-dimethylthiourea	64.20	63.70	63.05
168	2-methylbutane	64.40	63.07	62.37
169	p-hydroquinone	64.70	61.65	61.57
170	N,N'-dimethylthiourea	64.70	64.80	63.75
171	methylacetylacetone	65.00	74.33	74.22
172	dibromomethane	65.10	71.45	71.05
173	isopropyl bromide	65.10	65.40	64.89
174	n-propyl bromide	65.60	68.02	66.62
175	trichloroethylene	65.80	62.51	61.57
176	n-butyl formate	65.83	66.50	66.18
177	2,3-dimethyl-2-butene	65.90	69.51	67.76
178	n-propyl acetate	65.91	68.18	67.15
179	m-nitrosonitrobenzene	66.00	71.43	77.84
180	toluene	66.11	65.06	64.63
181	bromodichloromethane	66.30	68.43	68.83
182	2-methylthiophene	66.35	60.66	59.20
183	2,5-dimethylfuran	66.37	66.23	64.95
184	methyl butyrate	66.40	68.01	66.83
185	p-nitroaniline	66.43	68.93	74.36
186	pentanoic acid	66.50	66.27	66.18
187	ethyl propionate	66.50	68.93	67.77
188	carbon tetrachloride	66.60	67.45	68.79
189	phthalic anhydride	**66.70**	**80.27**	**81.93**
190	salicylaldehyde	66.80	68.68	69.24
191	p-hydroxybenzaldehyde	66.80	68.55	69.19
192	isopropyl acetate	67.04	68.72	67.32
193	n-butyl chloride	67.10	65.52	64.63
194	chloromaleic acid	67.38	66.67	66.94
195	N-propyl urea	67.40	63.13	63.43
196	n-amyl alcohol	67.50	65.79	64.98
197	5,5-dimethylcyclopentadiene	67.50	70.31	70.08
198	iso-valeric acid	67.70	66.15	65.98
199	phenylhydrazine	67.82	65.21	65.61
200	cyclohexane	68.13	69.86	70.26
201	styrene	68.20	69.38	69.03
202	phenylhydroxylamine	68.20	63.70	63.86
203	diethyl ketoxime	68.30	70.40	69.33
204	p-dinitrobenzene	68.30	73.22	83.63
205	methyl n-propyl ketone oxime	68.82	69.66	68.72
206	isoamyl alcohol	68.96	65.53	64.80
207	N-allylthiourea	69.00	67.02	66.70
208	ethyl n-propyl ketone	69.03	74.95	74.30
209	2-pentanol	69.10	66.72	65.49
210	cycloheptene	69.30	75.10	75.43
211	tetrahydrofurfuryl alcohol	69.40	66.60	66.46
212	hexanal	69.40	72.92	72.92
213	2,4-dimethylpyrrole	69.64	66.88	66.69
214	dimethyl malonate	69.69	72.37	71.14
215	benzaldoxime	69.80	70.65	71.06
216	tert-butyl methyl ketone	69.86	73.72	73.51

Table 2 (continued)

No	Compounds	$-\chi_M(10^{-6}cgs)$		
		Experimental	Calculated 1	Calculated 2
217	isobutyl methyl ketone	70.05	74.27	73.46
218	m-nitroaniline	70.09	68.96	74.36
219	1-butanethiol	70.20	71.30	67.86
220	benzoic acid	70.28	68.84	69.39
221	p-nitrosotoluene	70.40	73.52	74.32
222	m-phenylenediamine	70.40	64.72	65.09
223	m-dinitrobenzene	70.53	73.22	83.62
224	p-phenylenediamine	70.70	64.64	65.10
225	m-nitrophenol	70.80	67.46	72.59
226	phenylthiol	70.80	71.71	69.19
227	2,4-dimethylpyridine	71.30	74.39	73.92
228	cyclohexanone oxime	71.50	76.42	77.10
229	triquinoyl	71.60	72.33	76.51
230	isoamylamine	71.60	67.29	66.86
231	1,2-dibromoethylene	71.70	75.71	72.04
232	acetylthiophene	71.70	79.89	81.60
233	2,5-dimethylpyrrole	71.92	67.01	66.75
234	ethyl succinimide	72.00	78.02	79.40
235	acetophenone	72.05	76.83	76.87
236	2,3-heptadiene	72.10	75.28	73.93
237	o-nitrotoluene	72.20	75.49	80.14
238	*m-cresol*	72.20	69.65	69.06
239	ethyl chloroacetate	72.30	70.79	69.86
240	benzamide	72.30	70.35	71.15
241	fluoro trichloroethylene	72.50	65.17	64.67
242	2,6-dimethylpyridine	72.50	74.57	74.01
243	o-phenylenediamine	72.50	64.75	65.15
244	m-nitrotoluene	72.70	75.38	80.09
245	phenyl iso-cyanate	72.70	67.74	69.05
246	1,3-cyclooctadiene	72.80	80.55	80.80
247	o-cresol	72.90	69.67	69.12
248	trichloroacetaldehyde	73.00	65.56	66.90
249	trichloroacetic acid	73.00	70.38	71.51
250	methyl dichloroacetate	73.10	71.53	70.76
251	2,4-dinitrophenol	73.10	77.81	88.12
252	p-nitrotoluene	73.30	75.33	80.10
253	o-nitrophenol	73.30	67.54	72.65
254	phloroglucinol	73.40	66.27	66.00
255	isoamyl cyanide	73.40	71.58	71.67
256	1,2-heptadiene	73.50	73.49	72.55
257	1,5-pentanediol	73.50	67.98	67.43
258	erythritol	73.80	63.78	63.12
259	1-allylpyrrole	73.80	69.53	70.11
260	2-methylcyclohexanone	74.00	81.91	82.47
261	N,N'-diethylurea	74.10	76.85	76.49
262	1,4-dichloro-2-butyne	74.20	69.27	68.42
263	1,3,5-trinitrobenzene	74.55	83.51	99.10
264	n-hexane	74.60	74.81	73.76
265	*1-chloro-4-nitrobenzene*	74.70	76.95	81.90
266	3-methylcyclohexanone	74.80	81.63	82.20
267	salicylic acid	75.00	73.48	73.88
268	chlorodibromomethane	75.10	80.06	81.18
269	benzylamine	75.26	69.61	69.79
270	trichloronitromethane	75.30	65.02	70.25

Table 2 (continued)

No	Compounds	$-\chi_M(10^{-6}cgs)$		
		Experimental	Calculated 1	Calculated 2
271	1-chloro-2-nitrobenzene	75.50	77.13	81.93
272	3-methylpentane	75.52	75.04	73.93
273	N,N,N',N'-tetramethylurea	75.70	77.35	76.10
274	o-methoxybenzaldehyde	76.00	81.65	81.12
275	o-nitrobenzoic acid	76.11	79.24	84.91
276	2,3-dimethylbutane	76.22	74.23	73.56
277	n-amyl nitrate	76.40	76.84	80.95
278	m-xylene	76.56	77.66	76.55
279	p-chloroaniline	76.70	72.66	72.63
280	p-xylene	76.78	77.43	76.58
281	benzeneacetonitrile	76.90	73.95	74.60
282	1-heptyne	77.00	74.19	73.61
283	n-butyl bromide	77.14	80.02	77.78
284	o-aminobenzoic acid	77.18	75.00	75.65
285	1-chloro-3-nitrobenzene	77.20	77.01	81.89
286	Phenylfluoroform	77.30	71.75	73.18
287	n-butyl acetate	77.47	79.29	78.38
288	p-chlorophenol	77.60	71.17	70.87
289	o-xylene	77.68	77.59	76.62
290	ethyl n-butyrate	77.70	80.05	79.01
291	1-heptene	77.80	78.20	77.22
292	m-cresylmethyl ether	77.91	82.54	80.95
293	p-methoxybenzaldehyde	78.00	81.47	81.08
294	hexanoic acid	78.10	77.52	77.40
295	ethyl isobutyrate	78.32	80.18	79.09
296	cinnamic acid	78.36	85.49	85.92
297	*phthalimide*	78.40	81.10	83.70
298	glutamic acid	78.50	74.26	75.36
299	isobutyl acetate	78.52	79.05	78.21
300	2,4-dimethyl-2,4-hexadiene	78.70	87.14	84.56
301	cycloheptane	78.90	81.07	81.48
302	1,2-dibromoethane	78.90	83.87	81.92
303	bromobenzene	78.92	79.27	77.67
304	isoamyl chloride	79.00	76.75	75.65
305	n-hexyl alcohol	79.20	77.00	76.21
306	guaiacol	79.20	74.71	73.50
307	dipropyl ether	79.40	79.26	77.78
308	2-heptyne	79.50	75.98	74.82
309	isobutyl bromide	79.88	79.02	77.63
310	acetophenone oxime	79.90	83.36	83.15
311	methyl n-butyl ketone oxime	79.97	80.72	79.96
312	isopropenylbenzene	80.00	81.72	80.95
313	p-chlorotoluene	80.07	79.06	78.37
314	1,2-dichloro-2-hydroxypropane	80.10	69.70	69.44
315	m-nitrobenzoic acid	80.22	79.13	84.86
316	4-methyl-2-pentanol	80.40	77.94	76.51
317	di-n-propyl ketone	80.45	86.15	85.54
318	n-amyl methyl ketone	80.50	85.45	84.90
319	1,1-difluoro-2,2-dichloroethyl methyl ether	80.68	75.87	75.50
320	n-butyl ethyl ketone	80.73	86.05	85.54
321	phenyl-propiolic acid	81.00	82.15	82.87
322	heptyldehyde	81.02	84.13	84.15
323	dibromodichloromethane	81.10	89.36	92.10
324	1,2-dimethylcyclopentane	81.31	82.43	81.93

Table 2 (continued)

No	Compounds	$-\chi_M(10^{-6}$cgs)		
		Experimental	Calculated 1	Calculated 2
325	triethylamine	81.40	83.25	81.20
326	benzyl formate	81.43	79.85	80.15
327	phenyl isothiocyanate	81.50	79.59	80.00
328	phenyl thiocyanate	81.50	85.33	84.56
329	tetrachloroethylene	81.60	75.80	74.99
330	diethyl oxalate	81.70	85.67	84.76
331	ethyl methylacetoacetate	81.90	91.67	90.87
332	benzyl chloride	81.98	78.87	78.57
333	o-chlorotoluene	81.98	79.23	78.41
334	N-phenyl urea	82.10	76.38	77.88
335	2,3,5-trimethylpyrrole	82.31	79.65	78.73
336	p-toluic acid	82.40	81.23	81.34
337	coumarin	82.50	85.23	86.20
338	*2-nitroso-1-naphthol*	**82.70**	**98.41**	**99.81**
339	cyclohexanoneoxime-o-methyl ether	82.90	89.37	89.00
340	p-dichlorobenzene	82.93	80.68	80.17
341	indene	83.00	79.50	79.88
342	2,4,6-trimethylpyridine	83.10	87.28	85.93
343	phenyl methyl sulfide	83.20	91.17	89.34
344	cyclohexanecarboxylic acid	83.24	85.15	85.93
345	benzyl methyl ketone	83.44	87.59	87.64
346	o-chlorobenzoic acid	83.56	83.13	83.16
347	phthalic acid	83.60	85.23	86.14
348	propiophenone	83.73	88.67	88.74
349	1-nitroso-2-naphthol	**83.90**	**98.43**	**99.80**
350	isoquinoline	83.90	81.74	82.83
351	p-bromoaniline	84.06	85.21	83.89
352	methyl trichloroacetate	84.20	83.58	83.37
353	o-dichlorobenzene	84.26	80.86	80.20
354	1,6-hexanediol	84.30	79.19	78.66
355	o-toluic acid	84.30	81.48	81.37
356	*1-chloro-2,4-dinitrobenzene*	84.40	87.39	97.41
357	phenetole	84.50	82.12	81.19
358	isophthalic acid	84.60	85.06	86.09
359	xylose	84.80	74.74	74.79
360	leucine	84.90	82.72	82.74
361	iso-leucine	84.90	83.39	83.26
362	dihydronaphthalene	85.10	90.74	91.10
363	N,N-dimethylaniline	85.10	83.73	83.00
364	heptane	85.24	86.03	84.99
365	1,1-difluoro-2,2-dibromoethane	85.50	82.80	83.72
366	*N-ethylaniline*	85.60	83.54	83.19
367	arabinose	85.70	74.74	74.79
368	quinoline	86.00	81.87	82.93
369	3-ethylpentane	86.20	87.37	85.47
370	methyl salicylate	86.60	86.35	85.77
371	p-dimethoxybenzene	86.65	87.48	85.34
372	bromobenzene diazo cyanide	**86.88**	**100.45**	**100.35**
373	acetylphenylacetylene	86.90	90.06	90.36
374	2,2-dimethylpentane	86.97	85.57	84.35
375	chorodifluoromethylbenzol	87.20	82.82	83.44
376	cinnamyl alcohol	87.20	84.75	84.42
377	o-bromonitrobenzene	87.30	89.78	93.16
378	o-bromoaniline	87.32	85.41	83.92

Table 2 (continued)

No	Compounds	$-\chi_M(10^{-6}$cgs)		
		Experimental	Calculated 1	Calculated 2
379	N-phenylthiourea	87.40	88.56	88.92
380	2,4-dimethylpentane	87.48	86.20	84.56
381	o-methoxybenzyl alcohol	87.90	85.52	84.10
382	2-methylheptene	88.00	90.31	88.99
383	*2-methyl-4-heptene*	88.00	91.17	89.96
384	*biphenylene*	**88.00**	**101.27**	**101.95**
385	7-hydroxy-2h-chromen-2-one	88.22	89.74	90.64
386	methyl-m-hydroxybenzoate	88.40	86.26	85.72
387	phenylacetylchloride	88.50	89.23	89.43
388	isoamyl bromide	88.70	91.53	88.77
389	methyl-p-hydroxybenzoate	88.70	86.22	85.72
390	1-octene	88.80	89.42	88.45
391	tetrahydroquinoline	89.00	91.60	92.35
392	propylbenzene	89.10	88.21	87.72
393	p-chloroanisole	89.10	84.08	82.75
394	isoamyl acetate	89.40	90.26	89.43
395	propyl butyrate	89.40	91.01	90.28
396	3,3-dimethylpentane	89.50	85.88	84.96
397	isopropylbenzene[cumene]	89.50	88.38	87.78
398	1,1,2,2-tetrachloroethane	89.80	80.75	81.29
399	gallic acid	90.00	82.58	82.83
400	1,2-dibromo-1,1,2-trifluoroethane	90.90	86.50	85.24
401	azulene	91.00	85.19	85.56
402	ethyl cyclohexane	91.09	93.55	93.21
403	ethyl 3-methylbutanoate	91.10	91.03	90.05
404	adonitol	**91.30**	**78.67**	**77.89**
405	phthalamide	91.30	88.27	89.66
406	n-hexyl methyl ketone	91.40	96.66	96.13
407	4-heptanol	91.50	89.64	88.33
408	4-nitroso-l-naphthol	91.80	98.45	99.80
409	naphthalene	91.90	85.19	85.56
410	iodobenzene	92.00	89.79	84.99
411	propyl sulfide	92.10	99.88	97.40
412	acetophenone oxime-o-methyl ether	92.31	96.32	95.06
413	methyl perfluor-n-butyrate	92.50	83.77	86.30
414	diethyl malonate	92.60	96.49	95.50
415	methyl phenylacetate	92.73	92.47	92.04
416	diiodomethane	93.10	92.75	88.60
417	benzyl acetate	93.18	92.60	92.36
418	1,2,3,4-tetrahydronaphthalene	93.30	96.49	96.84
419	N-methyl-N'-phenylurea	93.35	89.26	90.32
420	amylidene chloride	93.40	89.14	88.66
421	4-phenyl-1-butene	93.49	91.52	91.19
422	phenyl propionate	93.79	93.72	93.71
423	ethyl benzoate	93.80	93.72	93.46
424	ethyl ethylacetoacetate	93.90	100.47	99.40
425	2,3-dibromo-2-butene-1,4-diol	94.20	103.55	100.05
426	phenyl ethyl sulfide	94.40	100.67	98.96
427	2,5-dimethyl-1-ethylpyrrole	94.61	91.91	90.64
428	propionylphenylacetylene	95.10	101.78	102.24
429	amylene chloride	95.20	83.71	82.54
430	2-butene-1,4-diyl diacetate(cis)	95.20	96.75	97.44
431	l-butene-3,4-diyl diacetate	95.50	100.06	98.83
432	ethylacetophenone	95.50	99.79	99.98

Table 2 (continued)

No	Compounds	$-\chi_M(10^{-6}$cgs)		
		Experimental	Calculated 1	Calculated 2
433	3,7,7-trimethyl-1,3,5-cycloheptatriene	95.60	99.38	98.62
434	methyl-o-methoxybenzoate	95.60	99.32	97.65
435	2-butyne-1,4-diyl diacetate	95.90	96.80	95.98
436	1,1-difluoro-2,2-dichloroethyl ethyl ether	96.13	87.88	87.68
437	8-methylquinoline	96.57	94.52	94.92
438	2-naphthol	96.80	89.71	90.00
439	p-phenetidine	96.80	88.11	87.40
440	4-methylheptane	97.30	98.11	96.34
441	6-methylquinoline	97.43	94.34	94.88
442	2-benzylidenemalonic acid	97.50	101.76	102.69
443	ethyl iodoacetate	97.60	97.08	91.54
444	7-methylquinoline	97.86	94.31	94.88
445	benzylidene chloride	97.90	91.72	91.64
446	*d-limonene*	98.00	104.42	103.28
447	2-naphthalenamine	98.00	91.22	91.77
448	2,5-dimethylhexane	98.15	96.77	95.85
449	1-nitronaphthalene	98.47	95.58	101.08
450	6-hydroxy-4-methyl-2h-chromen-2-one	98.69	102.41	102.62
451	2,3-dimethylhexane	98.77	97.83	96.32
452	3,4-dimethylhexane	99.06	98.45	96.67
453	pentachloroethane	99.10	92.69	93.84
454	rhamnose	**99.20**	**86.99**	**86.70**
455	p-chloroiodobenzene	99.42	103.73	98.74
456	octanoic acid	99.50	99.94	99.86
459	2-methylquinoline	99.86	94.49	94.97
460	7-hydroxy-4-methyl-2h-chromen-2-one	99.96	102.42	102.62
461	1-nonene	100.10	100.63	99.68
462	2,5-dimethyl-4-heptene	100.60	103.34	101.82
463	n-butylbenzene	100.79	99.30	98.96
464	durene	101.20	102.78	100.53
465	p-iodotoluene	101.31	102.10	96.94
466	*dimethyl terephthalate*	101.60	110.79	109.88
467	*o-phenetidine*	**101.70**	**88.24**	**87.45**
468	isoamyl propionate	101.73	101.97	101.31
469	eugenol	102.10	102.40	100.78
470	tert-butylbenzene	102.50	99.25	98.75
471	glucose	**102.60**	**89.59**	**89.55**
472	isopropylcyclohexane	102.65	104.96	104.39
473	octyl alcohol	102.65	99.43	98.67
474	2-methylnaphthalene	102.70	97.65	97.50
475	*p-cymene*	102.80	100.76	99.73
476	1-methylnaphthalene	102.90	97.87	97.54
477	mannose	**102.90**	**89.59**	**89.55**
478	camphor	103.00	114.91	114.18
479	biphenyl	103.25	101.87	102.16
480	1-acetyl-1-(ethyloxylcarbonyl)cyclobutane	103.40	110.95	111.12
481	ethyl perfluor-n-butyrate	103.50	95.76	98.49
482	di-n-butylamine	103.70	103.09	102.46
483	di-tert-butyl ketone	104.06	108.87	107.56
484	ethyl phenylpropiolate	104.20	106.96	106.95
485	diisobutyl ketone	104.30	108.23	107.61
486	ethylene iodide	104.70	107.33	99.07
488	dimethyltrichloromethylcarbinol	105.00	92.91	93.28
489	diethyl succinate	105.00	107.67	106.72

Table 2 (continued)

No	Compounds	$-\chi_M(10^{-6}$cgs)		
		Experimental	Calculated 1	Calculated 2
490	7,8-dihydroxy-4-methyl-2h-chromen-2-one	105.10	107.10	107.18
491	dipropyl oxalate	105.27	107.61	107.29
492	(e)-2-(3-phenylallylidene)malonic acid	**105.40**	**118.43**	**119.29**
493	phenyl n-butyrate	105.46	104.85	104.95
494	6-hydroxy-5-nitro-4-methylcoumarin	105.60	112.90	118.19
495	diisobutylamine	105.70	102.75	102.09
496	di-sec-butylamine	105.90	104.81	103.32
497	7-hydroxy-4-methyl-8-nitro-2h-chromen-2-one	106.00	112.86	118.20
498	2,5-dimethyl-3-propyl-pyrrole	106.07	102.85	101.81
499	4,6-dimethylcoumarin	106.20	110.35	110.13
500	*benzil*	**106.80**	**125.07**	**126.70**
501	azobenzene	106.80	112.00	113.65
502	cis-decahydronaphthalene	107.00	112.70	112.81
503	1-methoxynaphthalene	107.00	102.80	101.94
504	ethyl cinnamate	107.50	110.34	110.00
505	*trans-decahydronaphthalene*	107.60	112.70	112.81
506	2-methoxynaphthalene	107.60	102.61	101.89
508	sorbitol	**107.80**	**93.51**	**92.65**
509	N,N-diethylaniline	107.90	108.25	107.00
510	p-tert-butylphenol	108.00	103.74	103.20
511	xanthone	108.10	117.92	119.20
512	n-nonane	108.13	108.45	107.44
514	1,2-dichloro-1,2-dibromoethane	108.60	105.83	105.52
515	2-nitrobiphenyl	109.00	112.26	117.68
516	*carvacrol*	109.10	105.38	104.23
517	Naphthalene-1-thiol	109.50	104.62	102.10
518	6-methoxy-4-methylcoumarin	109.50	115.31	114.51
519	4-methyloctane	109.63	109.15	107.58
520	diphenylamine	109.70	107.72	108.91
521	1,1-di(ethyloxylcarbonyl)cyclopropane	110.40	116.31	116.52
522	fluorene	110.50	112.21	112.70
523	N-nitrosodiphenylamine	110.70	116.68	118.91
524	benzidine	110.90	113.86	114.58
525	acenaphthylene	111.60	101.29	101.89
526	ethyl-1-methyl-2-oxocyclohexanecarboxylate	112.10	122.32	122.36
527	m-iodotoluene	112.30	102.72	96.89
529	ethyl amylpropiolate	112.70	115.66	114.94
530	1,6-dimethylnaphthalene	113.30	110.34	109.48
531	diethyl tartrate	113.40	115.23	114.22
532	5-hydroxy-4,7-dimethylcoumarin	113.50	115.10	114.61
533	1-phenyl-2-methylbutane	113.53	110.92	110.35
534	n-butyl sulfide	113.70	122.77	119.82
535	amylene bromide	114.50	107.70	105.33
536	ethyl nitrophenylpropionate	114.60	125.06	130.13
538	phenothiazine	114.80	126.60	129.41
539	ethyl p-toluenesulfonate	115.00	113.42	114.07
540	diphenyl diazomethane	115.00	119.99	121.38
541	n-octyl mercaptan	115.10	116.04	112.78
542	diethyl ethylmalonate	115.20	120.48	119.04
543	diphenylmethane	115.70	112.61	112.93
544	5-nitroacenaphthylene	116.00	111.65	117.41
545	benzyl butyrate	116.30	115.45	115.49
546	ethyl benzylidenecyanoacetate	116.30	120.94	121.24
547	2,4'-dinitrobiphenyl	116.50	122.54	133.15
548	n-butyl benzoate	116.69	115.81	115.96

Table 2 (continued)

No	Compounds	$-\chi_M(10^{-6}$cgs)		
		Experimental	Calculated 1	Calculated 2
549	diisobutylmethanol	116.90	111.86	110.40
550	triiodomethane	117.10	117.71	118.18
552	N-2-naphthylacetamide	117.80	115.90	116.49
553	1,2,3-tribromopropane	117.90	122.61	118.34
554	1,1-diphenylethylene	118.00	118.54	118.48
555	1,1-di(ethyloxylcarbonyl)cyclobutane	118.00	127.77	127.72
557	anthrone	118.00	123.76	124.97
558	aminoazobenzene	118.30	118.12	119.91
559	busulphan	118.68	121.34	124.15
560	diethyl allylmalonate	118.80	123.82	122.52
561	acridine	118.80	114.49	115.93
562	valerylphenylacetylene	119.00	124.06	124.71
563	7,7'-bis(cycloheptatrienyl)	119.00	122.67	123.00
564	diphenylsulfane	119.20	121.16	122.91
565	2-ethoxynaphthalene	119.20	114.66	114.07
566	decane	119.50	119.67	118.67
567	anthraquinone	119.60	124.57	126.49
568	1-ethoxynaphthalene	119.90	114.82	114.12
569	carbazole	**119.90**	**107.19**	**108.70**
570	flavone	**120.00**	**134.49**	**135.74**
571	p-methyl-o-tert-butyl-phenol	120.30	116.44	115.18
572	ethyl 1-isobutylacetoacetate	121.40	125.50	124.77
573	2-naphthalenesulfonylchloride	121.91	118.69	121.21
574	dimethylallylacetophenone	122.40	126.58	126.27
575	N,N,N',N'-tetraethylurea	122.40	126.05	124.14
576	ethylally acetophenone	122.50	126.74	126.61
577	4-aminostilbene	122.50	124.36	124.92
578	*N-phenylbenzothioamide*	123.00	131.75	132.19
579	cinnamylideneaniline	123.20	131.79	132.68
580	1,1,2,2-tetrabromoethane	123.40	129.77	130.03
581	1-bromonaphthalene	123.60	112.31	110.56
582	cytidine	123.70	126.51	128.83
583	n-hexyl benzene	124.23	121.75	121.41
584	diethylcyclohexylamine	124.50	124.79	123.47
585	n-amyl valerate	124.55	124.52	123.97
586	diisopropylbenzene	124.77	124.61	122.90
587	triethyl phosphate	**125.30**	**110.51**	**107.19**
588	chalcone	125.70	130.02	130.98
590	chrysoidine	126.30	124.16	126.12
591	N,N-diphenyl urea	126.30	125.94	127.63
592	n-butyl perfluor-n-butyrate	126.70	117.85	120.99
593	cyclododecene	127.00	131.17	131.57
594	m,m'-bitolyl	127.40	126.85	126.04
596	1,2-diphenylethane	127.80	123.83	124.15
597	m-azotoluene	127.80	136.97	137.53
598	Pentyl benzoate	128.50	127.07	127.19
599	tetra(chloromethyl)methane	129.00	119.31	116.76
600	camphoric acid	129.00	118.84	117.83
601	isoamyl ether	129.00	123.38	122.34
602	pentachlorohexadione	129.50	139.37	140.83
603	1,1-difluoro-2,2-dichloroethyl amyl ether	129.84	121.21	121.41
604	ethyl hexylpropiolate	129.90	126.87	126.17
605	anthracene	**130.00**	**117.74**	**118.45**
606	stilbestrol	130.00	127.36	127.60
607	caproylphenylacetylene	130.40	135.31	135.94

Table 2 (continued)

No	Compounds	$-\chi_M(10^{-6}$cgs)		
		Experimental	Calculated 1	Calculated 2
608	(e)-1-benzylidene-1h-indene	130.50	134.45	135.04
609	7-phenylbenzofulvene	131.00	134.67	134.80
610	*Dibenzyl ketone*	131.70	135.02	135.95
611	chlorodiphenylmethane	131.90	126.86	126.74
612	tryptophan	**132.00**	**118.01**	**119.98**
614	N,N,N',N'-tetraethylthiourea	132.60	138.36	135.09
615	4,4'-dichlorobiphenyl	133.10	129.90	129.65
616	methylethylallylacetophenone	133.30	138.72	138.06
617	n-heptyl benzene	134.41	132.97	132.64
618	4,5-dimethylnonane	134.52	132.34	130.34
619	diphenyldiacetylene	134.60	128.26	129.14
620	3,4-dimethylnonane	134.70	132.16	130.35
621	benzoic anhydride	134.90	130.16	131.68
622	azotoluene	135.10	136.78	137.55
623	diethyl ketone-2,4-dinitrophenylhydrazone	135.16	141.99	152.09
624	2,5-dimethyl-2,5-dibromo-3-hexyne	135.60	136.06	135.44
625	tetraiodomethane	136.00	139.81	147.29
628	1-phenylazo-2-naphthol	137.60	149.30	151.08
629	4-ethoxy-3-methoxybenzyl acetate	138.50	139.64	137.25
630	phenanthrenonitrile	139.00	128.60	129.72
632	ethyl diethylmalonate	140.40	144.67	142.36
633	1-phenyl-4-benzoyl-1,3-butadiene	140.80	146.72	147.57
634	acetoaminofluorene	141.00	142.57	143.16
635	anthracenenitrile	**142.10**	**128.41**	**129.67**
636	9-cyanoanthracene	**142.10**	**128.58**	**129.72**
637	ethyl phenylmalonate	142.20	145.23	144.54
638	chloromethylstilbene	144.80	144.92	144.64
639	perhydroanthracene	146.01	155.42	155.39
640	1,1-diphenylallyl-3-chloride	146.10	143.80	143.28
641	9-methylanthracene	**146.50**	**130.67**	**130.46**
642	diphenylhexatriene	146.90	152.21	151.75
643	hexachlorobenzene	147.00	138.59	135.28
644	ethyl diallyl acetophenone	147.40	154.50	153.32
645	9-butylidene-9h-fluorene	147.50	153.86	153.73
646	dodecyl alcohol	147.70	144.28	143.58
647	pyrene	**147.90**	**134.01**	**134.82**
648	m-nitro carbanilide	148.10	145.91	158.86
649	di-n-hexylamine	148.90	148.02	147.37
650	N,N'-dimethyl-N,N'-diphenylurea	148.90	150.25	151.72
651	perfluorobutyric anhydride	**149.40**	**134.24**	**141.72**
652	*o-terphenyl*	150.40	151.31	151.68
653	Octylene bromide	150.40	152.10	149.20
654	*p-terphenyl*	152.00	151.09	151.64
655	Ethyl ethylpropylmalonate	152.40	155.97	153.59
656	9-ethyl anthracene	153.00	142.68	142.31
657	ethyl methylphenylmalonate	153.20	157.42	156.21
658	methyldiphenoxyphosphine oxide	153.90	144.25	143.67
659	2-methylcarbanilide	**154.00**	**137.89**	**139.91**
661	Methyldiphenyltriazine	155.10	154.40	156.06
662	m-terphenyl	155.50	151.11	151.64
663	triphenylene	156.60	150.87	151.46
664	tri-iso-butylamine	156.80	149.89	148.05
665	3,4-bis-(p-hydroxy-phenyl)-2,4-hexadiene	**157.00**	**170.67**	**168.83**
666	l-(p-tolylazo)-2-naphthol	157.60	161.69	163.03
667	octylcyclohexane	158.09	160.85	160.58

Table 2 (continued)

No	Compounds	$-\chi_M(10^{-6}cgs)$		
		Experimental	Calculated 1	Calculated 2
668	9-methyl-10-methoxy anthracene	158.10	148.42	146.89
669	o-(2,5-dimethoxybenzoyl)-benzoicacid	161.00	164.86	163.90
670	9-methyl-3,4-benzoacridine	161.10	159.64	160.81
671	*l-(p-chloro phenylazo)-2-naphthol*	161.40	163.31	164.82
672	triethyl citrate	161.90	162.91	161.51
673	l-(o-methoxyphenylazo)-2-naphthol	163.60	166.86	167.46
674	9-propylanthracene	164.00	153.78	153.56
675	tetraiodoethylene	164.30	161.37	150.51
676	5-cyclohexylacenaphthene	165.20	172.79	173.36
677	2,6-di-tert-bntyl-4-methyl phenol	165.30	163.30	161.29
678	tetradecane	166.20	164.52	163.58
679	chrysene	**166.67**	**150.67**	**151.42**
680	tetracene	**168.00**	**150.30**	**151.33**
681	2-butyne-1,4-dibenzoate	169.00	169.36	170.64
682	methyl n-hexyl ketone-2, 4-dinitrophenylhydrazone	171.73	174.78	185.17
683	1,6-diphenylhexane	171.81	168.70	169.06
685	ethyl dibromocinnamate	174.50	164.36	160.06
686	*triphenylcarbinol*	175.70	166.00	166.05
687	9-butyl anthracene	176.00	164.88	164.79
688	N,N',N-triphenyl urea	176.60	174.86	177.67
689	diethyl sebacate	177.00	174.90	174.09
690	2-phenyl-5,7-dimethylpleiapentalene	179.00	175.95	175.33
691	*diphenyldecapentaene*	180.50	185.58	184.94
692	methylcholanthrene	182.00	184.56	184.80
693	5,7,9-trimethyl-3,4-benzoacridine	183.70	185.18	184.80
694	1,2,5,6-dibenzofluorene	184.00	177.72	178.55
695	acenaphthanthracene	184.00	174.50	175.78
696	5,7,9-trimethyl-1,2-benzoacridine	184.50	188.56	187.70
697	hexadecane	187.60	186.94	186.03
698	tetraiodopyrrole	188.90	194.63	171.82
699	sugar	189.10	178.49	177.44
700	2,2,4,7,9,9-hexamethyldecane	191.52	187.57	185.04
701	*dibenz[a,h]anthracene*	193.00	183.21	184.30
702	3-methylcholanthrene	194.00	185.04	185.14
703	5,7,8,9-tetramethyl-3,4-benzoacridine	196.30	198.06	196.82
704	dibenzphenanthrone	200.50	189.53	190.86
705	4,4'-diphenylbiphenyl	201.30	200.30	201.12
706	1,1-diphenylnonane	206.32	204.18	203.81
707	cis-9-octadecenoic acid	208.50	206.11	206.08
708	5,11-dibromotetracene	216.00	205.38	201.34
709	tetraphenylethylene	217.40	217.45	217.80
710	tri-n-hexylamine	221.70	217.29	216.02
711	1,1,4,4-tetraphenylbuta-1,2,3-triene	227.00	230.41	231.31
712	n,n,n',n'-tetraphenylthiourea	229.70	236.60	238.39
713	1,1-dicyclohexylnonane	231.98	237.74	236.97
714	tetraphenylhexatriene	246.40	251.10	250.80
715	tri-n-heptylamine	251.30	250.93	249.70
716	diethylstilbestrol dipropionate	**265.20**	**250.19**	**248.46**
717	pyranthrene	**266.90**	**248.27**	**249.93**
718	violanthrene	**273.50**	**286.40**	**287.93**
719	cholic acid	282.30	284.35	280.99
720	cholesterol	**284.20**	**302.50**	**298.54**
721	dicetyl sulfide	401.70	391.70	389.30

Table 3 Experimental and calculated diamagnetic susceptibilities of 360 organic compounds (test set). Compounds with standard deviations larger than two standard errors are in bold

No	Compound	$-\chi_M(10^{-6}$cgs)		
		Experimental	Calculated 1	Calculated 2
722	formaldehyde	18.60	15.07	14.80
723	nitromethane	21.10	25.31	30.27
724	formamide	21.90	21.33	21.48
725	allene	25.30	26.86	25.80
726	ethane	27.30	31.32	29.69
727	methyl formate	31.10	32.41	31.50
728	methyl chloride	32.00	33.50	32.21
729	cyanogen chloride	32.40	28.43	28.02
730	acetone	33.70	40.04	39.35
731	vinyl formate	34.70	36.93	36.38
732	maleic anhydride	35.80	47.62	48.93
733	pyrazine	37.80	45.91	47.20
734	propionitrile	38.50	38.40	38.15
735	ethylene glycol	38.90	34.54	33.73
736	cyclopropane	39.90	35.45	36.65
737	propane	40.50	41.15	40.09
738	difluoroacetamide	41.20	37.35	38.74
739	thiourea	42.40	38.93	38.91
740	methyl acetate	42.60	45.09	43.71
741	oxalic acid	42.90	35.97	36.60
742	Ethyl hydroxylamine	43.00	38.91	38.15
743	*trans-2-butene*	43.30	45.95	44.38
744	2-methylpropene	44.40	44.74	43.46
745	cyclopentadiene	44.50	46.97	47.12
746	1-nitropropane	45.00	48.76	53.58
747	cyclopropanecarboxylic acid	45.33	50.68	52.32
748	2-nitropropane	45.73	49.45	53.73
749	n-butyraldehyde	46.08	50.48	50.47
750	vinyl acetate	46.40	49.70	48.59
751	ethanethiol	47.00	48.44	45.47
752	succinimide	47.30	54.26	56.14
753	2-chloropropene	47.80	46.30	45.27
754	fulvene	48.00	52.48	52.35
755	4-hydroxy-2-butanone	48.50	54.05	53.66
756	1,4-cyclohexadiene	48.70	58.02	58.15
757	trans-1,2-dichloroethylene	48.90	49.37	48.19
758	fumaric acid	49.10	52.60	53.13
759	cyclopentene	49.50	52.69	52.97
760	1,3-propylene glycol	50.20	45.59	44.98
761	thiazole	50.55	52.57	55.21
762	methylfumaric acid	**50.98**	**65.05**	**65.14**
763	isobutane	51.70	51.46	50.79
764	tetronic acid	52.50	52.35	53.68
765	chloroacetylchloride	53.70	55.20	55.11
766	2-methyl-2-butene	54.14	57.67	56.05
767	ethyl bromide	54.70	56.74	55.46
768	benzene	54.84	52.63	52.68
769	bromochloromethane	55.00	58.43	57.60
770	morpholine	55.00	57.83	58.06
771	1,5-hexadiene	55.10	59.19	58.23
772	ethyl thiocyanate	55.70	61.48	60.63
773	1-methoxy-1,1,2-trifluoroethane	55.90	50.47	50.48
774	isobutyric acid	56.06	55.15	55.03
775	n-butyl alcohol	56.54	54.53	53.76

Table 3 (continued)

No	Compound	$-\chi_M(10^{-6}cgs)$		
		Experimental	Calculated 1	Calculated 2
776	Piperazine	56.80	59.40	60.27
777	3,4-dimethyloxadiazole	57.17	62.21	61.71
778	dimethyl furazan	57.27	59.81	60.00
779	ethyl methyl ketoxime	57.30	58.28	57.50
780	methyl n-propyl ketone	57.41	63.14	62.43
781	iso-valeraldehyde	57.50	61.41	61.52
783	isobutyl alcohol	57.70	54.18	53.59
784	methyl chloroacetate	58.10	58.77	57.68
785	cyclobutanecarboxylic acid	58.16	61.93	63.55
786	methyl isopropyl ketone	58.45	62.99	62.53
787	1-bromo-2-propene	58.60	60.57	58.80
788	ethyl iso-thiocyanate	59.00	54.77	54.15
789	chloroform	59.30	56.23	56.62
790	1,2-dichloroethane	59.60	55.81	55.54
791	4-methylpyridine	59.80	61.62	61.89
792	1,1-dichlorodifluoroethylene	60.00	54.18	54.45
793	2-methylpyridine	60.30	61.85	61.98
794	*p-nitrosophenol*	60.70	65.63	66.82
795	furfuryl alcohol	61.00	56.33	56.00
796	1,3-cycloheptadiene	61.00	69.35	69.57
797	1,4-butanediol	61.50	56.76	56.21
798	ethyl oxamate	62.00	62.32	62.44
799	dimethyl sulfate	62.20	57.02	56.68
800	ethyl thiolacetate	**62.70**	**75.21**	**73.72**
801	n-pentane	63.05	63.64	62.53
802	ethyl thionacetate	63.50	68.73	66.96
803	aspartic acid	64.20	63.09	64.13
804	piperidine	64.20	64.57	65.27
805	1-hexyne	64.50	62.95	62.39
806	1,3,5-cyclooctatriene	65.10	74.84	74.94
807	benzonitrile	65.19	63.15	63.86
808	p-nitrosonitrobenzene	65.80	71.42	77.85
809	o-dinitrobenzene	65.98	73.30	83.67
810	1,2-dichloro-1,1,2-trifluoroethane	66.20	61.07	61.96
811	uric acid	66.20	77.21	83.07
812	1-hexene	66.40	66.97	66.00
813	o-nitroaniline	66.47	69.04	74.41
814	p-nitrobenzaldehyde	66.57	74.33	80.22
815	isobutyl formate	66.79	66.31	66.00
816	chlorofumaric acid	67.02	66.67	66.94
817	ethyl cyanoacetate	67.30	65.95	65.88
818	2-n-butyl chloride	67.40	64.69	64.30
819	tartric acid	67.50	65.42	66.08
820	diethyl sulfide	67.90	76.75	75.05
821	o-nitrobenzaldehyde	68.23	74.45	80.27
822	m-nitrobenzaldehyde	68.55	74.35	80.22
823	dichloroacetyl chloride	69.00	67.88	68.19
824	methyl butyl ketone	69.10	74.20	73.68
825	n-amylamine	69.40	67.50	67.05
826	asparagines	69.50	64.60	65.89
827	p-nitrophenol	69.50	67.44	72.60
828	ethyl iodide	69.70	68.28	64.07
829	chlorobenzene	69.97	66.69	66.42
830	methylcyclopentane	70.17	70.43	70.40

Table 3 (continued)

No	Compound	$-\chi_M(10^{-6}cgs)$		
		Experimental	Calculated 1	Calculated 2
831	2,4-pentanediol	70.40	69.78	68.46
833	tert-amyl alcohol	70.90	66.32	65.52
834	1,5-cyclooctadiene	71.50	80.42	80.60
835	ethyl acetoacetate	71.70	79.49	78.93
836	benzyl alcohol	71.83	67.89	67.73
837	phenylacetylene	72.01	65.52	65.61
838	phenylacetaldehyde	72.01	75.05	75.66
839	p-toluidine	72.10	71.04	70.84
840	anisole	72.20	70.07	69.01
841	*p-cresol*	72.40	69.54	69.07
842	ethyl lactate	72.60	72.15	71.04
843	1-iodo-2-propene	72.80	72.39	67.35
844	thiobarbituric acid	72.90	73.04	74.94
845	bromotrichloromethane	73.10	78.65	80.39
846	Benzylidenemethylamine	73.10	75.46	75.46
847	cyclohexanol	73.40	73.31	73.62
848	cyclopentanecarboxylic acid	73.48	73.93	74.70
849	5-methyl-1,2-hexadiene	73.60	73.25	72.37
850	n-methylaniline	74.10	71.68	71.30
851	valine	74.30	71.56	71.69
852	m-toluidine	74.60	71.17	70.82
853	cinnamic aldehyde	74.80	80.83	81.33
854	2-methylpentane	75.26	74.83	73.55
855	diethyl carbonate	75.40	74.03	72.49
856	benzoyl chloride	75.60	78.48	78.66
857	o-toluidine	76.00	71.17	70.88
858	2,2-dimethylbutane	76.24	73.58	73.19
859	m-chloroaniline	76.60	72.81	72.62
860	Saligenin(salicylalcohol)	76.90	72.52	72.22
861	methyl bromoacetate	77.10	73.14	70.81
862	ethylbenzene	77.20	76.99	76.48
863	o-chlorophenol	77.40	71.31	70.91
864	m-chlorophenol	77.60	71.29	70.86
865	propyl propionate	77.70	79.89	79.03
866	1-chloro-2,3-dihydroxypropane	**77.90**	**59.78**	**59.23**
867	1,2-dibromo-2-fluoroethane	78.00	84.27	82.47
868	phenyl-propylnitrile	78.20	85.18	85.82
869	isoamyl formate	78.38	77.47	77.22
870	hydrindene	78.50	85.30	85.61
871	p-nitrobenzoic acid	78.81	79.12	84.86
872	methylcyclohexane	78.91	81.64	81.63
873	p-cresylmethyl ether	79.13	82.46	80.96
874	n-butyl thiocyanate	79.38	84.50	83.01
875	o-chloroaniline	79.50	72.81	72.68
876	m-anisidine	79.95	76.11	75.21
877	m-chlorotoluene	80.07	79.31	78.35
878	1,3-dichloro-2-hydroxypropane	80.10	70.81	70.07
879	o-anisidine	80.44	76.22	75.27
880	p-anisidine	80.56	76.06	75.22
881	perfluoro-n-butyric acid	81.00	70.88	74.41
882	diisopropyl ketone	81.14	86.78	85.65
883	1,1-diethoxyethane	81.40	85.58	82.70
884	dimethyl succinate	81.50	83.58	82.36
885	methyl benzoate	81.60	81.72	81.28
886	o-cresylmethyl ether	81.94	82.71	80.99

Table 3 (continued)

No	Compound	$-\chi_M(10^{-6}cgs)$		
		Experimental	Calculated 1	Calculated 2
887	phenyl acetate	82.04	82.05	81.82
888	benzeneacetic acid	82.40	79.64	80.14
889	bromoform	82.60	91.13	93.66
890	ethyl bromoacetate	82.80	85.11	83.00
891	m-toluic acid	83.00	81.33	81.33
892	m-dichlorobenzene	83.19	80.97	80.14
893	phenyl propiplamide	83.30	95.03	95.49
894	1,2-octadiene	83.60	84.73	83.78
895	trifluoro cresol	83.80	78.95	79.80
896	nitrophenyl fluoroform	84.10	82.15	88.70
897	n-propyl iodide	84.30	79.75	75.20
898	picric acid	84.38	88.18	103.65
899	cyclooctene	84.60	86.32	86.66
900	dimethylcyclohexanone	84.80	93.26	93.63
901	m-bromoaniline	84.89	85.47	83.86
902	indole	85.00	74.39	75.70
903	ethyl dichloroacetate	85.20	83.48	82.95
904	benzylideneaminoethane	85.50	90.22	90.24
905	phenylbutadiene	85.70	86.09	85.63
906	2-methylhexane	86.24	85.84	84.80
907	diethyl sulfate	86.80	81.26	81.01
908	2-ethylbutyrylchloride	87.20	88.83	87.44
909	m-dimethoxybenzene	87.21	87.50	85.34
910	o-dimethoxybenzene	87.39	87.66	85.39
911	2,3-dimethylpentane	87.51	86.44	85.11
912	p-fluorophenetole	88.00	85.11	84.69
913	2,2,3-trimethylbutane	88.36	84.93	84.47
915	p-bromotoluene	88.70	91.61	89.63
916	n-amyl acetate	89.06	90.55	89.61
917	butyl propanoate	89.10	91.01	90.27
918	m-bromonitrobenzene	89.50	89.61	93.13
920	m-phenetidine	90.28	88.16	87.39
921	benzylideneamino-1-hydroxylethane	91.00	93.54	93.60
922	methyl amyl ketone oxime	91.24	91.97	91.19
923	cyclooctane	91.40	92.29	92.71
924	triethylphosphine oxide	91.60	96.30	95.00
926	carvone	**92.20**	**104.80**	**104.32**
927	1,3,5-trimethylbenzene	92.30	90.42	88.47
928	1-naphthalenamine	92.50	91.36	91.82
929	n-heptylamine	93.10	89.93	89.51
930	m-bromotoluene	93.40	92.06	89.58
931	n-butyl iodide	93.60	92.14	86.33
932	thia coumarin	93.60	103.49	102.78
933	carbon tetrabromide	**93.73**	**109.31**	**115.90**
934	2,5-dimethyl-3-ethyl-pyrrole	93.87	91.71	90.57
935	4-meth ylquinoline	94.71	94.50	94.92
936	benzoyl acetone	95.00	99.20	99.91
937	1-naphthol	95.22	89.84	90.06
938	methyl phenylpropiolate	95.60	94.94	94.76
939	anethole	96.00	99.70	97.86
940	n-octane	96.63	97.24	96.22
941	dimethylacetophenone	96.80	100.02	100.05
942	2,2-di(chloromethyl)propane	96.90	89.65	89.14
943	safrole	97.50	100.31	99.93
944	3-ethylhexane	97.80	98.64	96.70

Table 3 (continued)

No	Compound	$-\chi_M(10^{-6}cgs)$		
		Experimental	Calculated 1	Calculated 2
945	3-methylheptane	97.99	97.60	96.38
946	2,2,4-trimethylpentane	98.34	97.10	95.35
947	methyl-p-methoxybenzoate	98.60	99.14	97.61
948	citral	98.90	107.73	106.52
949	fluorenone	**99.40**	**113.00**	**114.21**
950	ethyl trichloroacetate	99.60	95.49	95.57
951	3-methyl-3-ethylpentane	99.90	98.48	96.70
952	benzylidene aniline	**100.40**	**115.05**	**116.08**
953	hexyl acetate	100.90	101.77	100.83
954	p-dibromobenzene	101.40	105.78	102.68
955	pseudocumene	101.60	90.13	88.55
956	isobutylbenzene	101.81	99.26	98.76
957	n-hexyl methyl ketoxime	102.58	103.18	102.42
958	fructose	**102.60**	**90.20**	**89.97**
959	octanone oxime	102.70	101.92	101.70
960	2,5-dimethyl-3-hexyne-2,5-diol	103.00	94.75	93.58
961	galactose	**103.00**	**89.59**	**89.55**
962	butane-1,4-diyl diacetate	103.40	106.29	105.45
963	hexylpropiolamide	103.70	103.54	103.85
964	ethyl phenylacetate	104.27	104.53	104.21
965	triethyl phosphite	**104.80**	**119.60**	**115.43**
966	n-propyl benzoate	105.00	104.69	104.73
967	tyrosine	105.30	100.58	101.36
968	7-hydroxy-4-methyl-6-nitro-2h-chromen-2-one	105.50	112.77	118.15
969	ethyl propylacetoacetate	105.70	114.80	113.69
970	di-iso-propyl oxalate	106.02	108.48	107.65
972	1,3,5-trichlorobenzene	106.50	95.45	93.84
973	5,7-dihydroxy-4-methylcoumarin	106.90	107.14	107.11
974	1,1-difluoro-2,2-dichloroethyl propyl ether	107.19	98.83	98.95
975	1-chloronaphthalene	107.60	99.53	99.33
976	nitrotri(chlormethyl)methane	107.80	102.97	106.34
977	diphenyl ether	108.10	106.90	107.13
978	trimethyl acetophenone	108.20	110.85	111.02
979	2,6-dimethyl-2,6,8-nonatriene	108.80	113.08	110.81
980	acenaphthene	109.30	106.86	107.31
981	benzophenone	109.60	113.46	114.43
982	1-iodo-2-phenylacetylene	110.10	103.63	98.24
983	7-methoxy-4-methyl-2h-chromen-2-one	110.50	115.32	114.51
984	5-methyl-5-nonene	111.60	114.88	113.23
985	o-iodotoluene	112.20	102.38	96.96
986	hexachloroethane	112.70	104.75	106.43
987	nicotine	113.33	111.18	111.79
988	isoamyl n-butyrate	113.52	113.10	112.56
989	1,1,1-tri(chloromethyl)ethane	114.00	104.27	102.97
990	aminomethyldiethyldiazine	114.80	112.45	112.27
991	octyl chloride	114.90	110.32	109.54
992	tert-butylcyclohexane	115.09	115.87	115.28
993	ethyl benzoylacetate	115.30	116.18	116.48
994	diphenylacetylene	116.00	114.97	115.66
995	oenanthylidene chloride	116.50	111.59	111.12
996	2,6-dimethyl-4-hexanol	**116.90**	**100.75**	**99.37**
997	n-1-naphthylacetamide	117.80	116.05	116.54
998	ethyl diethylacetoacetate	117.90	127.95	125.75
999	naphthalene-1,2-dithiol	118.00	123.88	118.64
1000	diphenylmethanethione	118.10	125.38	125.44

Table 3 (continued)

No	Compound	$-\chi_M(10^{-6}cgs)$		
		Experimental	Calculated 1	Calculated 2
1001	amyl iodide	**118.75**	**103.04**	**97.58**
1002	p-methoxyazobenzene	118.90	129.42	129.98
1003	*diphenylmethanol*	119.10	116.66	116.86
1004	1,1-difluoro-2,2-dichloroethyl butyl ether	119.48	109.95	110.19
1005	ethyl tribromoacetate	119.50	128.90	130.42
1006	geraniol formate	119.90	123.61	122.03
1007	stilbene	120.00	118.37	118.71
1008	4-methylnonane	121.39	120.38	118.81
1009	camphane amine	122.00	120.12	118.66
1010	hexamethylbenzene	122.50	128.55	124.56
1011	2,6-dimethyloctane	122.54	119.88	118.64
1012	salol	123.20	123.16	123.90
1013	ethyl methyl ketone-2,4-dinitrophenylhydrazone	124.11	129.89	140.26
1014	diphenyl acetic acid	124.50	128.54	129.16
1015	9-ethylidene-9h-fluorene	124.80	131.33	130.83
1016	borneol	126.00	118.46	116.78
1017	N,N'-diethyl-N'-phenylurea	126.40	125.77	126.13
1018	3-bromo-7-hydroxy-4-methyl-2h-chromen-2-one	127.30	129.33	127.69
1019	N,N'-diphenyl urea	127.50	125.31	127.92
1020	phenanthrene	127.90	117.93	118.49
1021	phenylsulfone	129.00	120.88	123.22
1022	dicyclohexyl	129.31	135.13	135.27
1023	diphenylbutadiene	129.60	135.54	135.15
1024	diphenyldihydrotetrazine	129.90	140.37	143.88
1025	1,4-diphenylbutadiene	130.00	135.07	135.31
1026	2-phenyl bensofuran	130.50	122.84	123.48
1027	undecane	131.80	130.88	129.90
1028	*methylbenzylaniline*	132.20	131.50	131.46
1029	diisoamylamine	133.10	125.05	124.55
1030	phenylbutyl acetate	134.50	126.28	126.03
1031	2,4-dimethylnonane	134.68	131.64	129.82
1032	N,N-diphenylthiourea	134.90	137.76	138.65
1033	acepleiadiene	135.00	139.56	140.24
1034	methyl n-propyl ketone-2,4-dinitrophenylhydrazone	135.70	141.26	151.48
1035	fluoranthene	138.00	134.20	134.86
1036	ethyl butylmalonate	139.30	142.82	141.52
1037	methyl-o-benzoylbenzoate	139.40	142.71	143.08
1038	1,3-diphenylallyl-3-chloride	140.70	143.62	143.41
1039	aminoazotoluene	142.20	142.92	143.80
1040	benzyl 2-phenylacetate	143.70	139.92	140.69
1041	hexachlorohexatrione	145.00	152.85	155.20
1042	diethylallylacetophenone	146.20	151.18	149.84
1043	heptylcyclohexane	147.40	149.63	149.35
1044	methyl n-butyl ketone-2,4-dinitrophenylhydrazone	147.65	152.32	162.72
1046	3-nitrocarbanilide	**148.10**	**135.60**	**143.39**
1047	1-(o-tolylazo)-2-naphthol	**148.70**	**161.86**	**163.07**
1048	4,4'-dichloro-2,2'-dinitrobiphenyl	150.00	150.72	160.68
1049	4,4'-dibromobiphenyl	151.30	154.99	152.16
1050	tri allyl acetophenone	152.50	157.88	156.80
1051	tridecane	153.70	153.31	152.36
1052	anthracenedinitrile	**154.60**	**139.05**	**140.90**
1053	2,4-di-tert-butylphenol	155.60	150.56	149.31
1054	methyl amyl ketone-2,4-dinitrophenylhydrazone	156.84	163.56	173.94
1055	*biphenyl-4-yl(phenyl)methanone*	158.00	162.68	163.91
1056	l-(o-chloro phenylazo)-2-naphthol	161.00	163.50	164.86

Table 3 (continued)

No	Compound	$-\chi_M(10^{-6}cgs)$		
		Experimental	Calculated 1	Calculated 2
1057	aurin	161.40	171.88	172.78
1058	ethyl ethylbutylmalonate	163.30	167.01	164.84
1059	diphenyl octatetraene	164.30	168.89	168.35
1060	triphenylmethane	165.60	161.67	161.93
1061	perylene	166.80	166.96	167.79
1062	di-n-heptylamine	171.50	170.44	169.82
1063	piethylstilbestrol	172.00	177.06	175.28
1064	dibutyl phthalate	175.10	179.15	179.29
1065	tetradecanoic acid	176.00	167.22	167.22
1066	4-ethoxy-3-methoxybenzyl benzoate	177.30	176.17	174.83
1067	1-hexadecanol	183.50	189.13	188.49
1068	triphenyl phosphite	183.70	194.49	193.16
1069	1,2,5,6-dibenzoacridine	186.40	179.89	181.79
1070	estradiol	186.60	191.74	190.53
1071	tri-iso-amylamine	192.00	182.69	181.80
1072	pentabromophenol	194.00	193.78	182.02
1073	hexadecanoic acid	198.60	189.64	189.68
1074	tri anilino phosphine oxide	**201.70**	**189.46**	**190.89**
1075	dibenzopyrene	**213.60**	**199.65**	**200.72**
1076	octadecanoic acid	220.80	212.08	212.13
1077	tetraphenylbutadiene	228.00	234.13	234.12
1078	anthrazine	245.70	241.71	245.05
1079	tetraphenyloctatetraene	264.10	267.76	267.40
1080	tetraphenyl decapentaene	280.80	284.44	283.99
1081	hexabenzo[bc,ef,hi,kl,no,qr]coronene	346.00	346.43	348.51

partial least-squares regression, and principal component regression. In this study, we applied stepwise multivariate regression analysis to select significant descriptors for linear QSPR models.

In order to obtain validated QSPR models, the dataset was divided into two datasets: training set and test set. The training and test sets represented 66.67% (721 data points) and 33.33% (360 data points), respectively, of the data. Ideally, this division is performed such that points representing both the training and test set are distributed within the whole descriptor space occupied by the entire data set, and each point of the test set is close to at least one point of the training set. *k*-Means cluster analysis (*k*-MCA) performed using SPSS was used to split the set of compounds to guarantee this distribution [50–54]. A *k*-MCA splits the 1,081 organic compounds into seven clusters with 255, 406, 6, 280, 98, 31 and 5 members, with a standard deviation of 1.08, 0.93, 5.00, 1.31, 1.73, 2.37 and 6.47, respectively. The main results of the *k*-MCA for the 1,081 organic compounds are depicted in Table 4. Selection of the training and prediction set was carried out by randomly taking compounds belong to each cluster.

Linear regression analysis was carried out using SPSS. The regression of molar diamagnetic susceptibilities,

Table 4 The main results of the *k*-means cluster analysis (*k*-MCA) for the 1,081 organic compounds

Variance analysis				
Molecular connectivity index	Between SS[a]	Within SS[b]	Fisher ratio (F)	*P*-level[c]
$^0\chi'$	1,304.09	0.66	1,981.81	0.00
$^1\chi'$	529.15	0.32	1,680.30	0.00
$^2\chi'$	475.84	0.49	968.67	0.00
$^4\chi_p'$	122.42	0.20	617.80	0.00

[a] Variability between groups
[b] Variability within groups
[c] Level of significance

χ_m, versus ${}^0\chi'$, ${}^1\chi'$, ${}^2\chi'$, ${}^3\chi'_p$, ${}^3\chi'_c$, ${}^4\chi'_p$, ${}^4\chi'_c$ ${}^5\chi'_p$, ${}^4\chi'_{pc}$, and ${}^5\chi'_{pc}$ of 721 compounds (training set) resulted in a good 4-parameter model with a correlation coefficient, r , of 0.9918. The model can be depicted as follows:

$$\begin{aligned} &-\chi_m \times 10^{-6}(cgs) = 2.58 + 10.22\,{}^0\chi' \\ &+ 8.31\,{}^1\chi' - 1.19^2\chi + 1.45^4\chi'_p \\ &n = 721,\ r = 0.9918,\ r^2 = 0.9837,\ s = 5.56\,cgs, \\ &F = 10779.5,\ AIC = 31.32,\ FIT = 58.51 \end{aligned} \tag{8}$$

where n is the number of organic compounds included in the model, r is the correlation coefficient, r^2 is the square of the correlation coefficient, s is the standard deviation of the regression, F is the Fisher ratio, AIC is Akaike's information criterion [55, 56], and FIT is the KUbinyi function [55, 56].

The results calculated from Eq. 8 for 721 organic compounds are shown in Table 2 (Calculated 1). Finally, to test the prediction ability of the model (Eq. 8), the molar diamagnetic susceptibilities of another 360 compounds (test set) were calculated from the model (Eq. 8) and are listed in Table 3 (Calculated 1). A plot of calculated molar diamagnetic susceptibility versus experimental data is shown in Fig. 1.

Results and discussion

From the definition of δ'_i, we can see that the δ'_i values of the carbon are the same as the orginal atomic connectivity index for alkane, because E_i =12.625 when the carbon is sp^3 hybird. Therefore, we can use the definition to denote the delta values of all atoms. As we modified only the delta values (δ_i) of the molecular connectivity index, our new valence molecular connectivity indexes for alkane are the same as the original molecular connectivity indexes. The δ'_i defined in this paper differ for different atoms due to various electron numbers, valence electron numbers, and valence orbital energy. For the different atom groups of an atom in the same valences, δ'_i values are unequal due to different h_i or E_i. For example, both h_i are 2, so δ^v_i is 2 for both "ssCH2" and "dCH2". However, as the E_i values are 12.625, and 13.067, the δ'_i are 2.0000, and 2.0700, respectively. This shows that the definition of our new δ'_i value can reflect the different chemical environment of a given atom. The δ'_i of a skeletal atom expresses both electronic and topological information. At the same time, from the definition of the novel connectivity index ${}^m\chi'$, we find that the basic features of original molecular connectivity indexes are maintained in our novel valence molecular connectivity indexes. Thus our novel valence molecular connectivity indexes preserve features of the original molecular connectivity indexes that may be useful for QSAR and QSPR studies.

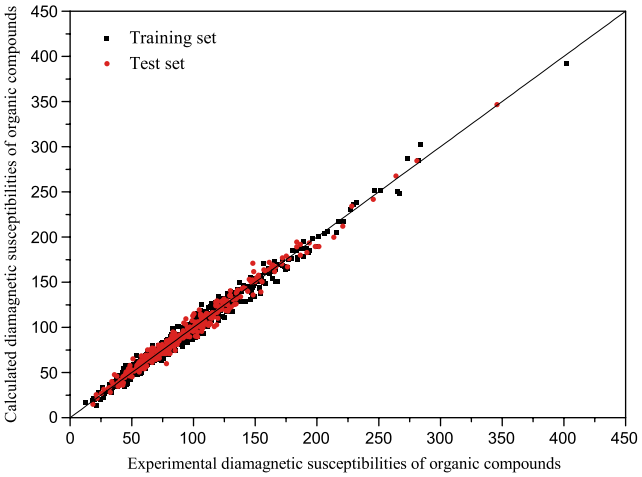

Fig. 1 Plot of calculated vs experimental values of molar diamagnetic susceptibilities, multivariate linear regression (MLR) model (Eq. 8)

The diamagnetic susceptibilities of various organic compounds have been investigated using the connectivity indices of Kier et al. [31] or the topological substructural molecular design approach of Estrada et al. [25–27]. In most cases, up to seven different kinds of indices have been employed to obtain a good linear fit to the experimental data. However, the large families of variables used in the correlation require more experimental χ_m values, which may not be available in practice.

The diamagnetic property of a compound is determined mainly by its molecular structure. Different compounds have different molecular structures, namely, different adjacency matrix of molecular graphs, and their ${}^m\chi'$ values are different. Based on Eq. 7, ${}^0\chi'$ is the sum of atomic δ'_i square root of the organic compound chemical formula, and ${}^1\chi'$ is the sum of chemical bonds of the chemical formula. So ${}^0\chi'$ and ${}^1\chi'$ contain atomic and bond contributions to the diamagnetic susceptibility of the compound.

The results of multivariate regression analysis have shown that the linear model (Eq. 8) is a good fit, and the correlation coefficient r is 0.9918. The model (Eq. 8) explains more than 98.37% of the variance in the experimental values of molar diamagnetic susceptibilities, χ_m, for these organic compounds. Because the coefficients may be influenced by two distant points, i.e., the numbers 721 and 1,081, we calculated the coefficients without them in order to see the real correlations. The correlation coefficient, r, and the square of the correlation coefficient, r^2, are 0.9913 and 0.9825 for 720 organic compounds. The results show that the coefficients are only slightly influenced.

From Tables 2 and 3, it can be seen that there are 51 compounds with standard deviations larger than two standard errors. The greatest errors in this data set are

recorded for some of the polyhalogenated compounds and polycyclic aromatic hydrocarbons (PAHs). For instance, the present approach gives errors of 23.02 and −18.63 cgs for hexabromoethane and pyranthrene, respectively. This result agrees with methods in the literature [27]. The theoretical prediction of the molar diamagnetic susceptibility of an organic compound is a complicated task that requires information from the levels of electron, atom, and molecule. Obviously, the limiting factor here is not in the use of a particular QSPR method but rather in the use of molecular descriptors that fail to account for all the details of the underlying system.

As shown in Table 2 (Calculated 1), our calculated values agree well with available experimental values. The average absolute deviation of 721 organic compounds (training set) is 4.26 cgs. The model was verified by cross-validation using the leave-one-out method, and the correlation coefficients r_{cv} and standard deviations s_{cv}, together with the normal r and s are 0.9916 (0.9918), 5.61 (5.56) cgs, respectively. The results of cross-validation of the model are very close to the normal results of the model, confirming the stability of the model constructed in this work. Finally, to test the prediction ability of the model (Eq. 8), the molar diamagnetic susceptibilities of another 360 organic compounds were calculated from the model (Eq. 8) and are listed in Table 3 (Calculated 1). This external prediction set includes amino acids, phosphate, sulfates, carbohydrates, heterocycles, and polycyclic aromatic compounds. Despite this degree of difficulty, the predicted values agree well with experimental values, and the average absolute deviation is 4.34 cgs. The plot of calculated molar diamagnetic susceptibility versus experimental data is shown in Fig. 1.

To allow comparison with original molecular connectivity indexes, the ${}^0\chi, {}^1\chi, {}^2\chi$ and ${}^4\chi_p$ were calculated and regressed with the molar diamagnetic susceptibilities (χ_m) of 721 organic compounds (training set). The result of regression is as follows:

$$\begin{aligned} &-\chi_m \times 10^{-6}(cgs) = 2.89 + 7.75\,{}^0\chi \\ &+ 11.30\,{}^1\chi + 0.35\,{}^2\chi - 0.14\,{}^4\chi_p \\ &n = 721,\ r = 0.9898,\ r^2 = 0.9797,\ s = 6.20\,cgs, \\ &F = 8639.0,\ AIC = 38.98,\ FIT = 46.89 \end{aligned} \tag{9}$$

The results calculated from Eq. 9 for 721 organic compounds are shown in Table 2 (Calculated 2), the average absolute deviation of 721 organic compounds (training set) is 4.65 cgs. To test the prediction ability of the model in Eq. 9, the molar diamagnetic susceptibilities of another 360 compounds were calculated from the model in Eq. 9, and are listed in Table 3 (Calculated 2); the average absolute deviation is 4.86 cgs. The plot of calculated molar diamagnetic susceptibility versus experimental data is shown in Fig. 2. Compared with the model in Eq. 9, the statistical parameters in the model in Eq. 8 improved with increases in the value of r, r^2, F, and FIT, and decreases in the value of s and AIC. The results show that our novel valence molecular connectivity indexes are more effective than the original molecular connectivity indexes for the prediction of the molar diamagnetic susceptibilities of organic compounds.

Using the topological substructural molecular design (TOSS-MODE) approach, Estrada et al. [27] developed two five-parameter models to estimate the diamagnetic susceptibilities of aliphatic and aromatic compounds. The correlation coefficient (r), the standard deviation (s), Akaike's information criterion (AIC), and the Kubinyi function (FIT) for the two models are 0.980, 0.980, 6.06 cgs, 3.82 cgs, 37.67, 44.93, 22.95, and 20.90, respectively. According to our method, if the diamagnetic susceptibilities of only the 233 aliphatic and 85 aromatic compounds from Ref. [27] are related to the novel molecular connectivities indexes, the two three-parameter models are shown as follows:

$$\begin{aligned} &-\chi_m \times 10^{-6}(cgs) = -2.05 + 13.08\,{}^0\chi' \\ &+ 6.51\,{}^1\chi' - 3.35\,{}^2\chi' \\ &n = 233,\ r = 0.9895, r^2 = 0.9790,\ s = 4.40\,cgs, \\ &F = 3565.4,\ AIC = 20.01, FIT = 44.20 \end{aligned} \tag{10}$$

$$\begin{aligned} &-\chi_m \times 10^{-6}(cgs) = 11.48 + 5.48\,{}^0\chi' \\ &\quad + 12.23\,{}^1\chi' + 7.29\,{}^4\chi'_p \\ &n = 85,\ r = 0.9888,\ r^2 = 9776, s = 2.82\,cgs, \\ &F = 1180.5, AIC = 8.76, FIT = 37.67 \end{aligned} \tag{11}$$

The standard deviaton(s) are decreased by 27.23% and 26.18%, respectively, AIC values are decreased, and FIT

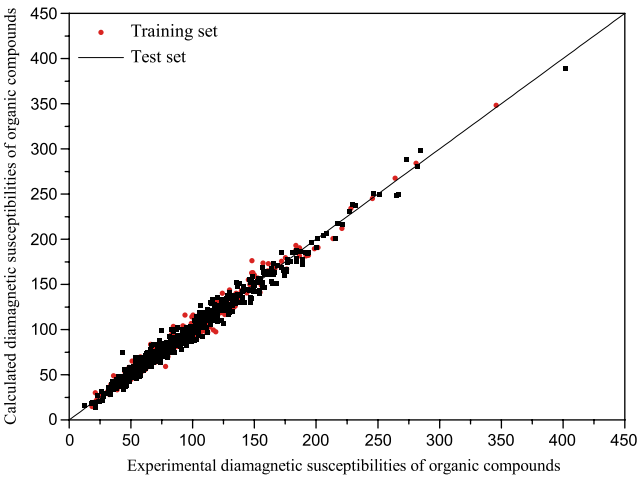

Fig. 2 Plot of calculated vs experimental values of molar diamagnetic susceptibilities, MLR model (Eq. 9)

values increased. The results show that the current method is more effective than the TOSS-MODE approach for the prediction of the molar diamagnetic susceptibilities of organic compounds.

Conclusion

A novel molecular connectivity index ${}^{m}\chi'$ for predicting the molar diamagnetic susceptibility of an inorganic compound, based on the adjacency matrix of molecular graphs and novel atomic valence connectivities, δ_i', has been proposed. A good QSPR model for molar diamagnetic susceptibilities can be constructed from ${}^{0}\chi', {}^{1}\chi', {}^{2}\chi'$, and ${}^{4}\chi_p'$, using MLR methods. The correlation coefficient *r*, standard error, and average absolute deviation of the MLR model are 0.9918, 5.56 cgs, and 4.26 cgs, respectively, for 721 organic compounds. Cross-validation using the leave-one-out method demonstrated that the MLR model is highly reliable from a statistical point of view. The average absolute deviations of predicted values of the molar diamagnetic susceptibility of another 360 organic compounds (test set) for the MLR model is 4.34 cgs. The results show that the method proposed here is more effective than literature methods for estimating the molar diamagnetic susceptibilities of organic compounds.

Acknowledgments This work is supported by the University Natural Science Foundation of Jiangsu Province in China (contract grant number: 04KJD150195). The authors express our gratitude to the referees for their value comments.

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