SHORT COMMUNICATION

MOLECULAR VOLUMES AND DENSITIES OF LIQUIDS AND SOLIDS BY MOLECULAR MECHANICS–ESTIMATION AND ANALYSIS

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Molecular volumes of 80 compounds (50 liquids and 30 solids), with densities in the range $0 \cdot 6-3 \cdot 0$ g cm^{-3}, were calculated by molecular mechanics. The densities derived from these molecular volumes ($V_{\text{mol MM}}$) by the approximation $d_{\text{MM}} = $ mol. wt/$V_{\text{mol MM}} N_A$ ($N_A = $ Avogadro's number) give two linear correlations (one for liquids and one for solids) when plotted versus experimental densities. Two general equations obtained from those relationships give a good precision (3% mean error) when tested in the calculation of the experimental densities of 183 compounds that have different structures and functional groups.

INTRODUCTION

Molecular volumes and densities are important parameters in physical organic chemistry.[1] They find applications in chemistry, biology and chemical engineering. Most of the methods of calculation used so far are empirical.[2-7] They are based either on elemental analysis (or on molecular weights) and correction factors for specific substructures (hydrogen-bonded functional groups, aromatic rings, etc.) or are incremental, using parameters characteristic of molecular fragments that are topological or at best defined by volumes derived from van der Waals radii (without taking into account the conformation of the molecule). These methods give acceptable predictions of densities but they have several limitations. They work reasonably well only within a series of molecules and they do not describe regioisomerism, steric strains or real conformations.

We were interested in the accurate prediction of densities of new organic compounds. This estimation at the molecular level is not easy since one needs both the molecular volume and the intermolecular volume (the free space between molecules). In principle, the molecular volume can be calculated accurately by theoretical methods (quantum mechanics or molecular mechanics). The intermolecular space can be obtained for crystals by sophisticated methods based on the crystalline arrangement of the solid, but this is lengthy and requires considerable computer investment.[8,9] Theoretical calculations of the intermolecular space are even more difficult for liquids.

We have developed a new method based on molecular mechanics which allows one to calculate the molecular volume, incorporates an average intermolecular volume and gives the density of liquids and solids directly. This method is simple, precise and valid for any new liquid or solid; in addition, the calculations can be carried out on a microcomputer.

RESULTS AND DISCUSSION

The calculations were carried out on 80 organic compounds (50 liquids and 30 solids)[10] selected so as to have a wide range of densities extending from 0·6 to 3·0 g cm^{-3}. The geometry of the conformation of minimum energy of each compound was obtained by molecular mechanics (MM) using the Allinger MM2 parametrization[11] with the EMO program.[12-16]

The molecular volume was then estimated in the following manner: the molecule in its minimum energy conformation was placed in a parallelepiped with each atom surrounded by the sphere corresponding to its MM van der Waals volume.[17] Successive and systematic testing of small fractions of the total volume of the parallelepiped (e.g. cubes having an edge 0·08 Å long), for the presence or absence of MM van der Waals volume leads to the molecular volume; the

smaller the cube, the more accurate the measure should be.[18-20]

From this molecular mechanics-calculated molecular volume ($V_{mol\ MM}$) one can estimate the density by taking

$$d_{MM} = \frac{\text{mol. wt}}{V_{mol\ MM}\ N_A}$$

where N_A = Avogadro's number. The value thus obtained should be considered as an overestimate since the intermolecular volume (V_{inter}) is not included the density of a liquid or a solid is

$$d = \frac{\text{mol. wt}}{(V_{mol} + V_{inter})\ N_A}$$

Indeed, the d_{MM} values reported in Table 1 are overestimated by 20–30% for low-density compounds (alkanes) and somewhat less (5–20%) for compounds having densities in the range 1–1·5 g cm^{-3}. In the case of high-density compounds ($d > 1·5$), on the other hand, d_{MM} is very close to d_{exp}[21] (except for polyhalo derivatives).

The mean deviation,

$$\frac{1}{N} \sum_1^N \frac{|d_{MM} - d_{exp}|}{d_{exp}} = 16.37\%$$

is much smaller than the usual mean difference between the molecular volume and the crystal volume; indeed, the packing coefficient k (molecular volume/crystal volume) is in the range 0·65–0·77 for most crystals

Table 1. Experimental and MM densities of 80 selected compounds (50 liquids and 30 solids)

Compound	Nature	d_{exp}[a]	d_{MM}	Deviation (%)[b]	Compound	Nature	d_{exp}[a]	d_{MM}	Deviation (%)[b]
Hexane	Liq.	0·659	0·874	32·63	Acetic acid	Sol.	1·266	1·308	3·32
Heptane	Liq.	0·683	0·887	29·87	1-Bromobutane	Liq.	1·276	1·592	24·78
1-Pentyne	Liq.	0·695	0·925	33·09	4-Acetylamino phenol	Sol.	1·293	1·372	6·11
Diethylamine	Liq.	0·707	0·925	30·83	Benzoic acid	Sol.	1·321	1·372	3·86
Diethyl ether	Liq.	0·714	0·963	34·87	Dichloromethane	Liq.	1·330	1·697	27·59
1-Decene	Liq.	0·742	0·932	25·61	2-Amino-5-nitrotoluene	Sol.	1·366	1·396	2·20
Dibutylamine	Liq.	0·760	0·948	24·74	4-Aminobenzoic acid	Sol.	1·374	1·422	3·49
Cyclohexane	Liq.	0·779	0·962	23·49	4-Chloroaniline	Sol.	1·429	1·436	0·49
Ethanol	Liq.	0·789	1·000	26·69	Bromoethane	Liq.	1·460	1·895	29·79
Acetone	Liq.	0·790	1·030	30·40	Maleic anhydride	Sol.	1·480	1·611	8·85
Methanol	Liq.	0·791	1·015	28·25	Nitric acid	Liq.	1·504	1·801	19·75
Propanal	Liq.	0·806	1·028	27·58	4-Chlorobenzoic acid	Sol.	1·541	1·562	1·36
Tetradecanoic acid	Sol.	0·862	1·048	21·55	2-Chloroacetic acid	Sol.	1·580	1·644	4·05
Cyclohexylamine	Liq.	0·867	1·045	20·53	Trinitromethane	Liq.	1·590	1·885	18·55
1,2-Diaminopropane	Liq.	0·874	1·052	20·37	1-Iodobutane	Liq.	1·615	2·006	24·18
Decanoic acid	Sol.	0·895	1·073	19·89	Tetranitromethane	Liq.	1·638	2·021	23·38
Ethyl formate	Liq.	0·923	1·177	27·52	2-dinitromethylene-1,3-diazacyclohexane	Sol.	1·666	1·541	7·50
1-Nitrohexane	Liq.	0·940	1·126	19·79	1,3,5-Trinitrobenzene	Sol.	1·680	1·741	3·63
Butanoic acid	Liq.	0·957	1·181	23·41	3-Methoxy-2,4,6-trinitroaniline	Sol.	1·710	1·755	2·63
Cyclohexanol	Sol.	0·960	1·086	13·13	2,4,6-Trinitroaniline	Sol.	1·762	1·788	1·48
Methyl formate	Liq.	0·974	1·230	26·28	N,N-Difluoro-2,4-dinitroaniline	Sol.	1·780	1·812	1·80
Benzylamine	Liq.	0·981	1·163	18·52	1,2-Dibromobutane	Liq.	1·791	2·132	19·01
Camphor	Sol.	0·992	1·146	15·52	Sulphuric acid	Liq.	1·827	2·017	10·40
Acetamide	Liq.	0·998	1·242	24·37	2,3,4,6-Tetranitroaniline	Sol.	1·870	1·876	0·32
Water	Liq.	1·000	1·234	23·40	Pyrosulphonic acid	Liq.	1·900	2·199	15·74
Propionic anhydride	Liq.	1·022	1·228	20·16	2-Bromobenzoic acid	Sol.	1·929	1·922	0·36
(2-Methylphenyl)methanol	Sol.	1·023	1·187	16·03	Bromochloromethane	Liq.	1·934	2·364	22·23
Benzaldehyde	Liq.	1·041	1·244	19·44	3-Trifluoromethyl-2,4,6-trinitroaniline	Sol.	1·936	1·986	2·58
Acetic acid	Liq.	1·050	1·308	24·67	Bromodichloromethane	Liq.	1·980	2·478	25·15
Acetic anhydride	Liq.	1·081	1·317	21·83	3-Bromo-2,4,6-trinitroanisole	Sol.	1·987	2·031	2·21
N-Acetylethanolamine	Sol.	1·108	1·245	12·37	*trans*-Difluorodinitroethylene	Sol.	2·048	2·051	0·15
Formamide	Liq.	1·133	1·356	19·64	3-Bromo-2,4,6-trinitroaniline	Sol.	2·157	2·140	0·79
Nitromethane	Liq.	1·137	1·363	19·88	1,2-Dibromoethane	Liq.	2·180	2·544	16·70
Acetamide	Sol.	1·159	1·242	7·16	1,4-Diiodobutane	Liq.	2·358	2·729	15·73
N-Acetyl-2-methylaniline	Sol.	1·168	1·228	5·14	1,2,3-Tribromopropane	Liq.	2·409	2·723	13·03
4-Chloroaniline	Liq.	1·169	1·436	22·84	Dibromochloromethane	Liq.	2·450	2·947	20·29
Benzyl phenyl ketone	Sol.	1·201	1·253	4·33	Dibromomethane	Liq.	2·496	2·929	17·35
Nitro benzene	Liq.	1·204	1·404	16·61	Tribromonitromethane	Liq.	2·793	3·226	15·50
N-Phenylacetamide	Sol.	1·210	1·255	3·68	1,1-Diiodoethane	Liq.	2·840	3·346	17·82
Methyl nitrate	Liq.	1·217	1·492	22·60	Tribromomethane	Liq.	2·887	3·361	16·42

[a] The experimental densities are taken from four references: A. J. Gordon and R. A. Ford, *The Chemist's Companion*, pp. 4–13. Wiley, New York (1972); *Guide de la Chimie International*. Chimidit, Paris (1992–93); Cambridge Structure Data Base (CRYSTAL); and S. Budavari *et al.* (Eds), *The Merck Index*, 11th ed. Merck, Rahway, NJ (1989).
[b] Deviation (%) = $(|d_{MM} - d_{exp}|/d_{exp}) \times 100$.

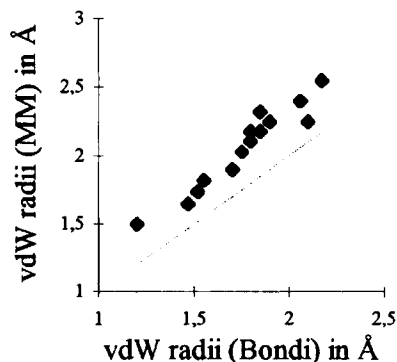Figure 1. Molecular mechanics van der Waals radii versus van der Waals radii according to Bondi

Figure 2. Molecular mechanics estimated density (d_{MM}) versus experimental density (d_{exp})

(or < 0.60 for most liquids) as determined by Kitaigorodsky.[22]

The good approximation of the density obtained from the MM molecular volume is thought to be due to the fact that van der Waals radii used in molecular mechanics calculations are larger than physical van der Waals radii (taken from Bondi[23]) by 0·2–0·4 Å. This difference, which has been discussed by Burkert and Allinger,[17] is shown clearly in Figure 1 for most of the atoms appearing in the molecular formulae in Table 1.

A close examination of densities calculated by molecular mechanics (d_{MM}) versus experimental densities in Figure 2 reveals one line for liquids and another for solids. The corresponding equations obtained from a least-squares fit are as follows:
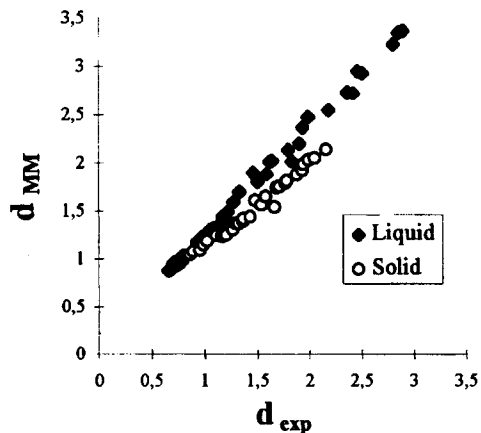
for liquids: $d_{MM} = 1·128 d_{exp} + 0·111$ $(r = 0·997)$

for solids: $d_{MM} = 0·873 d_{exp} + 0·244$ $(r = 0·990)$

The quality of these two correlations is surprisingly good; it can be expressed by a mean deviation, taken as

$$\frac{1}{N} \sum_{1}^{N} \frac{|d_{MM} - d_{\text{regression line}}|}{d_{\text{regression line}}}$$

of 2·37% for liquids and 2·42% for solids.

Keeping in mind that the MM molecular volume is larger than the physical molecular volume (since MM van der Waals radii are larger) and smaller than the
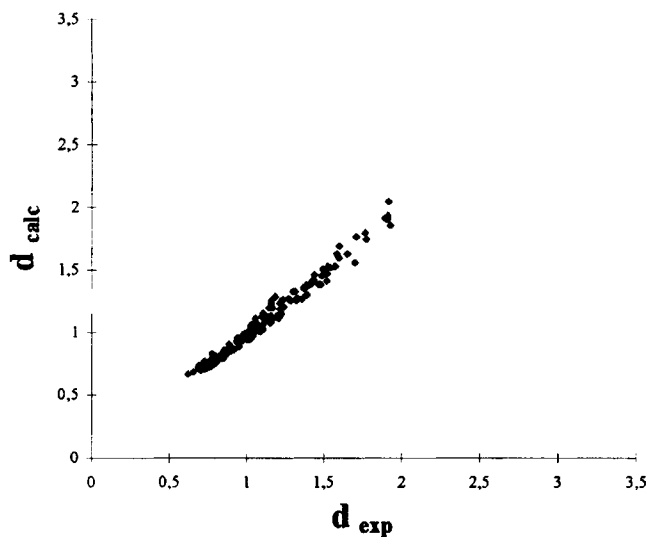

Figure 3. Calculated density (d_{calc}) versus experimental density (d_{exp})

crystal volume (which includes, in addition, the intermolecular volume), the slopes of the correlations can be interpreted differently for solids and liquids. For solids the slope smaller than unity (0·873) can be explained if we assume that crystals are more tightly packed for higher densities. In other words, the packing coefficient, k, is higher for high-density materials. In contrast, for liquids the slope larger than unity (1·128) can be understood if liquids are less tightly packed for high densities. In other words, the packing coefficient is smaller for high-density liquids.

In addition to these phenomenological observations, two general equations can be simply derived by reversing the two previous extrathermodynamic relationships; this gives an accurate estimated density value (d_{calc}) from the approximate density value

(d_{MM}) calculated directly from the MM molecular volume:

for liquids: $d_{calc} = 0·887 d_{MM} - 0·098$

for solids: $d_{calc} = 1·145 d_{MM} - 0·279$

These two equations were tested for predicting the densities of 183 compounds (143 liquids and 40 solids). The calculated (d_{calc}) and the experimental values (d_{exp}) are listed in Table 2 and plotted in Figure 3. The agreement is very good.[24] The correlation line corresponding to the least-squares fit is $d_{calc} = 0·995 d_{exp} - 0·010$ with $r = 0·993$; the mean error

$$\frac{1}{N} \sum_1^N \frac{|d_{calc} - d_{exp}|}{d_{exp}}$$

Table 2. Experimental, MM and calculated densities of 183 compounds

Compound	Nature	d_{exp}[a]	d_{MM}	d_{calc}	Error (%)[b]	Compound	Nature	d_{exp}[a]	d_{MM}	d_{calc}	Error (%)[b]
2-Methylbutane	Liq.	0·620	0·862	0·667	7·52	1-Propanol	Liq.	0·803	0·994	0·784	2·47
2-Methylpentane	Liq.	0·653	0·879	0·682	4·39	Pentylcyclohexane	Liq.	0·804	0·973	0·765	4·84
2,2,4-Trimethylpentane	Liq.	0·688	0·917	0·715	3·98	2-Butanone	Liq.	0·805	1·021	0·808	0·28
Isopropylamine	Liq.	0·689	0·938	0·734	6·53	2-Butanol	Liq.	0·807	0·994	0·784	2·89
Octane	Liq.	0·703	0·897	0·698	0·76	2-Pentanone	Liq.	0·809	1·013	0·801	1·03
2-Pentyne	Liq.	0·712	0·927	0·724	1·72	Pentanal	Liq.	0·809	1·011	0·799	1·33
4,4-Dimethylpentyne	Liq.	0·714	0·953	0·747	4·64	1-Butanol	Liq.	0·810	0·991	0·781	3·55
1-Hexyne	Liq.	0·715	0·933	0·730	2·04	Cyclohexene	Liq.	0·810	1·003	0·792	2·26
Nonane	Liq.	0·717	0·906	0·706	1·59	Cycloheptane	Liq.	0·811	0·978	0·769	5·12
2,7-Dimethyloctane	Liq.	0·725	0·920	0·718	0·96	2-Hexanone	Liq.	0·811	1·008	0·796	1·87
Di-isopropyl ether	Liq.	0·726	0·977	0·769	5·87	3-Hexanone	Liq.	0·812	1·009	0·797	1·83
Decane	Liq.	0·730	0·912	0·711	2·61	3-Pentanone	Liq.	0·814	1·014	0·801	1·52
2-Hexyne	Liq.	0·731	0·938	0·734	0·34	Hexanal	Liq.	0·814	1·006	0·794	2·41
1-Heptyne	Liq.	0·734	0·940	0·736	0·24	Butanal	Liq.	0·817	1·018	0·805	1·47
Undecane	Liq.	0·740	0·918	0·716	3·21	3-Methyl-2-Hexanone	Liq.	0·828	1·015	0·802	3·10
Cyclopentane	Liq.	0·745	0·948	0·743	0·29	Tetradecanoic acid	Liq.	0·844	1·048	0·832	1·46
1-Octyne	Liq.	0·746	0·945	0·740	0·78	Azetidine	Liq.	0·847	0·999	0·788	6·95
2-Heptyne	Liq.	0·748	0·942	0·738	1·40	1,1-Dimethoxyethane	Liq.	0·850	1·076	0·856	0·74
Dipropyl ether	Liq.	0·749	0·967	0·760	1·43	4,Isopropyltoluene	Liq.	0·857	1·044	0·828	3·38
Dodecane	Liq.	0·749	0·923	0·721	3·78	Methyl cyclopentyl ether	Liq.	0·862	1·057	0·840	2·60
Tridecane	Liq.	0·756	0·927	0·724	4·20	Cumene	Liq.	0·862	1·068	0·849	1·47
1-Nonyne	Liq.	0·758	0·948	0·743	2·00	1,3,5-Triethylbenzene	Liq.	0·863	1·031	0·816	5·39
1-Dodecene	Liq.	0·760	0·939	0·735	3·30	Mesitylene	Liq.	0·865	1·065	0·847	2·12
Methyl pentyl ether	Liq.	0·761	0·968	0·761	0·05	Ethylbenzene	Liq.	0·868	1·073	0·854	1·64
Ethyl pentyl ether	Liq.	0·762	0·969	0·762	0·07	Butyl propionate	Liq.	0·875	1·090	0·869	0·71
Tetradecane	Liq.	0·762	0·930	0·727	4·60	Methyl cyclohexyl ether	Liq.	0·875	1·056	0·839	4·15
Methylcyclohexane	Liq.	0·769	0·974	0·766	0·40	1-Chlorohexane	Liq.	0·878	1·095	0·873	0·54
Pentadecene	Liq.	0·769	0·933	0·730	5·13	1-Chlorobutane	Liq.	0·886	1·135	0·909	2·54
Dibutyl ether	Liq.	0·770	0·970	0·762	0·99	2,6-Di-*tert*-butyl-*p*-cresol	Liq.	0·894	1·114	0·890	0·40
Cyclopentene	Liq.	0·772	0·995	0·785	1·63	1,3,5-Triethylhexahydro-1,3,5-triazine	Liq.	0·894	1·111	0·887	0·73
Butyl methyl ether	Liq.	0·774	0·967	0·760	1·84	1,2-Diaminoethane	Liq.	0·898	1·070	0·851	5·22
Hexadecene	Liq.	0·774	0·936	0·732	5·40	1,3,5-Trimethylhexahydro-1,3,5-triazine	Liq.	0·919	1·084	0·864	6·04
Acetonitrile	Liq.	0·777	1·011	0·799	2·80	3-Methylbutyric acid	Liq.	0·933	1·159	0·930	0·32
1-Fluorobutane	Liq.	0·779	1·046	0·830	6·54	Methyl acetate	Liq.	0·939	1·187	0·955	1·69
Ethylcyclohexane	Liq.	0·784	0·972	0·764	2·53	Pentanoic acid	Liq.	0·939	1·149	0·921	1·91
2-Propanol	Liq.	0·785	0·996	0·785	0·01	Benzyl ethyl ether	Liq.	0·949	1·169	0·939	1·06
2-Methyl-2-propanol	Liq.	0·788	0·997	0·786	0·30	Cyclohexylbenzene	Liq.	0·950	1·111	0·887	6·58
1-Octadecene	Liq.	0·789	0·952	0·746	5·40	1-Nitropropane	Liq.	0·953	1·147	0·919	3·53
Propylcyclohexane	Liq.	0·790	0·973	0·765	3·16	Benzyl methyl ether	Liq.	0·963	1·197	0·964	0·04
Butylcyclohexane	Liq.	0·800	0·973	0·765	4·37	Butyric anhydride	Liq.	0·968	1·169	0·939	3·01
Isopropylcyclohexane	Liq.	0·802	0·980	0·771	3·83						
Isopentylcyclohexane	Liq.	0·802	0·978	0·769	4·05						

(continued)

Table 2. (Continued)

Compound	Nature	d_{exp}[a]	d_{MM}	d_{calc}	Error (%)[b]	Compound	Nature	d_{exp}[a]	d_{MM}	d_{calc}	Error (%)[b]
Cyclohexyl acetate	Liq.	0·970	1·161	0·932	3·94	Acetylformic acid	Liq.	1·227	1·467	1·203	1·95
1-Nitrobutane	Liq.	0·971	1·174	0·943	2·85	1,2-Dichloroethane	Liq.	1·235	1·535	1·264	2·31
4-Methylaniline	Liq.	0·973	1·169	0·939	3·50	1-(4-Chlorophenyl)-2-methyl-					
2,3-Butanedione	Liq.	0·981	1·223	0·987	0·61	2-propanol	Sol.	1·240	1·297	1·210	2·74
2-Nitropropane	Liq.	0·988	1·219	0·983	0·48	2,6-Dichlorotoluene	Liq.	1·269	1·547	1·274	0·41
Propionic acid	Liq.	0·993	1·229	0·992	0·09	1,1-Bis(propylamino)-2,2					
1-Phenyl-1-propanol	Liq.	0·994	1·192	0·959	3·47	-dinitroethylene	Sol.	1·275	1·356	1·270	0·11
Anisole	Liq.	0·996	1·181	0·950	4·67	4-Nitrotoluene	Sol.	1·287	1·344	1·260	2·11
1-Nitropropane	Liq.	1·001	1·215	0·980	2·13						
Hydrazine	Liq.	1·004	1·170	0·940	6·40	2-Chloro-4,6-bis(ethylamino)-s-					
Ethyl plenyl ketone	Liq.	1·009	1·184	0·952	5·68	triazine	Sol.	1·302	1·403	1·330	1·95
N-Methylformamide	Liq.	1·010	1·174	0·943	6·60	Maleic anhydride	Liq.	1·314	1·611	1·331	1·29
N-Acetylpiperidine	Sol.	1·011	1·130	1·010	0·38	2,4-Dinitrotoluene	Liq.	1·321	1·529	1·258	4·75
1-Phenylethanol	Liq.	1·015	1·181	0·950	6·48	Dimethyl sulphate	Liq.	1·328	1·548	1·275	3·99
1-Methylnaphthalene	Liq.	1·019	1·206	0·972	4·64	Adipic acid	Sol.	1·360	1·355	1·270	6·44
Aniline	Liq.	1·021	1·202	0·968	5·24	2-Chloroacetic acid	Liq.	1·370	1·644	1·360	0·74
2-Phenylethanol	Liq.	1·023	1·177	0·946	7·57	s-Triazine	Sol.	1·380	1·435	1·360	1·15
Acenaphthene	Liq.	1·024	1·256	1·016	0·79	4-Methoxybenzoic acid	Sol.	1·385	1·382	1·300	5·89
Butanoyl chloride	Liq.	1·028	1·298	1·053	2·46	Bromocyclopentane	Liq.	1·387	1·664	1·378	0·65
Isopropyl nitrate	Liq.	1·036	1·313	1·067	2·96	Trimethylene glycol 1,2,-					
Benzyl alcohol	Liq.	1·042	1·209	0·974	6·48	dinitrate	Liq.	1·393	1·581	1·304	6·36
4-Methylaniline	Sol.	1·046	1·169	1·060	1·29	4-Bromotoluene	Liq.	1·410	1·667	1·381	2·08
2,6-Di-tert-butyl-p-cresol	Sol.	1·048	1·114	1·000	4·91	4-Nitroaniline	Sol.	1·422	1·454	1·390	2·54
1-Nitroethane	Liq.	1·050	1·271	1·029	1·96	2-Bromotoluene	Liq.	1·425	1·699	1·409	1·12
Propionyl chloride	Liq.	1·056	1·367	1·115	5·54	1-Bromopropane	Liq.	1·435	1·714	1·422	0·88
Phenol	Liq.	1·057	1·256	1·016	3·93	1,1,2-Trichloroethane	Liq.	1·440	1·761	1·464	1·67
Allyl benzoate	Liq.	1·058	1·256	1·016	3·94	1-(Lactyl nitrate)glycerol					
Propyl nitrate	Liq.	1·058	1·306	1·060	0·23	dinitrate	Liq.	1·470	1·672	1·385	5·78
1-Chloro-4-fluorobutane	Liq.	1·063	1·312	1·066	0·29	Ethylene glycol dinitrate	Liq.	1·480	1·673	1·386	6·35
4-Chlorotoluene	Liq.	1·070	1·320	1·073	0·27	1-Bromo-4-chlorobutane	Liq.	1·488	1·753	1·457	2·09
Diphenyl ether	Liq.	1·075	1·267	1·026	4·57	3-Chlorobenzoic acid	Sol.	1·496	1·561	1·510	0·83
N,N-Methylphenylurethane	Liq.	1·090	1·245	1·006	7·68	Diglycerol dinitrate	Liq.	1·520	1·704	1·413	7·01
Ethyl nitrate	Liq.	1·100	1·384	1·130	2·69	2,4-Dinitrotoluene	Sol.	1·521	1·529	1·470	3·24
2-Fluoroethanol	Liq.	1·104	1·311	1·065	3·55	1,4-Dichlorobenzene	Sol.	1·526	1·584	1·530	0·57
(4-Methoxyphenyl)methanol	Sol.	1·109	1·257	1·160	4·62	2-Chlorobenzoic acid	Sol.	1·544	1·572	1·520	1·49
2-Acetoxyethanol	Liq.	1·109	1·270	1·028	7·28	2,4,6-Triamino-s-triazine	Sol.	1·573	1·581	1·530	2·65
4-Nitro toluene	Liq.	1·123	1·344	1·094	2·54	3,9-Bis(dinitromethylene)-					
Glyoxal	Liq.	1·140	1·376	1·123	1·53	2,4,8,10-tetraazaspiro					
Naphthalene	Sol.	1·145	1·228	1·130	1·57	[5·5]undecane	Sol.	1·587	1·671	1·630	2·98
Diphenyl ketone	Sol.	1·146	1·292	1·200	4·74	1,1,2,2-Tetrachloroethane	Liq.	1·595	1·929	1·613	1·13
Ethyl phenyl ketone	Sol.	1·157	1·396	1·080	6·94	Ethyl-(2,4,6-trinitrophenyl)					
2-Amino-5-nitro toluene	Liq.	1·159	1·396	1·140	1·62	carbamate	Sol.	1·600	1·640	1·600	0·08
Phenylnitromethane	Liq.	1·160	1·337	1·088	6·21	Isobutyl iodide	Liq.	1·602	2·021	1·695	5·78
(3-Hydroxyphenyl)methanol	Sol.	1·161	1·322	1·230	6·35	2,4,6-Trinitrotoluene	Sol.	1·654	1·665	1·630	1·61
2-Chloro-4,6-bis(isopropylamino)						2-(Dinitromethylene)-1,3-					
-s-triazine	Sol.	1·162	1·343	1·260	8·32	diazacyclopentane	Sol.	1·702	1·605	1·560	8·42
N-(2-Hydroxyethyl)						Picryl azide	Sol.	1·709	1·792	1·770	3·74
acetoacetamide	Sol.	1·168	1·291	1·200	2·67	Cyanuric acid	Sol.	1·768	1·813	1·800	1·63
2-Chloro-4-ethylamino-6-						2,4,6-Trinitrophenylhydrazine	Sol.	1·775	1·773	1·750	1·35
isopropylamino-s-triazine	Sol.	1·187	1·371	1·290	8·74	3,5-Dihydroxy-2,4,6-					
Dimethyl phthalate	Liq.	1·191	1·381	1·127	5·38	trinitroaniline	Sol.	1·896	1·924	1·920	1·48
2-Chloroethanol	Liq.	1·200	1·397	1·141	4·91	N,N-Difluoro-2,4,6-					
Propylene carbonate	Liq.	1·204	1·394	1·138	5·44	trinitroaniline	Sol.	1·910	1·911	1·910	0·05
N-Acetyl-4-methylaniline	Sol.	1·212	1·226	1·120	7·20	2,4,6-Trinitro-s-triazine	Sol.	1·915	1·942	1·940	1·55
2-Naphthol	Sol.	1·217	1·325	1·240	1·74	Tetrachlorophthalic anhydride	Sol.	1·920	2·037	2·050	6·95
Formic acid	Liq.	1·220	1·456	1·193	2·17	1,3,5-Triamino-2,4,6-					
1-Naphthol	Sol.	1·224	1·329	1·240	1·53	trinitrobenzene	Sol.	1·930	1·868	1·860	3·63
Acetanaphthene	Sol.	1·225	1·256	1·160	5·38	Diiodomethane	Liq.	3·325	3·811	3·282	1·29
Peracetic acid	Liq.	1·226	1·408	1·151	6·13						

[a] The experimental densities are taken from four references: A. J. Gordon and R. A. Ford, *The Chemist's Companion*, pp. 4–13. Wiley, New York (1972); *Guide de la Chimie International*. Chimidit, Paris (1992–93); Cambridge Structure Data Base (CRYSTAL); and S. Budavari *et al.* (Eds), *The Merck Index*, 11th ed. Merck, Rahway, NJ (1989).
[b] Deviation (%) = $(|d_{MM} - d_{exp}|/d_{exp}) \times 100$.

is 3·07%. This error is comparable to errors obtained with incremental methods within a limited series of parent compounds. It is smaller than the same error with incremental methods on enlarged series similar to those we have examined in this work. These enlarged series include groups with different skeletons and/or different functional groups.

CONCLUSION

The method of calculation described in this paper predicts the density of any organic compound directly from the molecular volume derived from molecular mechanics. The method is valid for liquids and solids. It gives a mean error of about 3%. It can be applied to any new material. In addition to this practical aspect, the results reported here may give interesting information on the molecular origin of the physical properties of liquids and solids.

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