x	mole fraction, liquid phase
x^{az}	azeotropic composition
y	mole fraction, vapor phase

Greek Letters

λ	parameter in eq 1
Δ	signifies a difference

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Density Estimations for Explosives and Related Compounds Using the Group Additivity Approach

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A first-order group additivity approach was used to estimate the densities of 188 explosives and related compounds of very diverse compositions. Of the 173 compounds for which direct comparisons could be made, 40.5% of the estimated densities were within 1% of the measured densities, 33.0% were within 1 to 2%, 16.8% were within 2 to 3%, and 9.8% deviated more than 3% from the measured densities. The average absolute error in density was 0.0191 g/cm^3, and the absolute error in density exceeded 0.05 g/cm^3 for only 14 of the 173 compounds (8.1%). The largest errors occurred for compounds with several bulky highly polar groups in close proximity and for compounds containing groups whose calculated molar volumes were based on density data for a small number of compounds. Inclusion of second-order effects, such as nearest neighbor interactions, phase transitions, and crystalline structure in a second-order group additivity model, appears necessary for accurate density estimations in certain types of compounds.

Introduction

As new families of organic compounds are identified for synthesis as potential high-energy explosives, a technique is required to estimate their steady-state detonation and metal acceleration properties. These estimated detonation parameters can then be compared with those measured for known explosives. Only the new molecules that offer significant advantages over currently used explosives would have to be synthesized and tested for their usefulness as explosives. A synthesis effort guided in this way would have the greatest probability of producing new, more powerful explosive molecules.

The main detonation property that determines the impulse delivered by an explosive is the Chapman–Jouguet (CJ) pressure, P_{CJ}, which is given by

$$P_{CJ} = \rho_0 D^2/(K + 1) \qquad (1)$$

where ρ_0 is the initial density of the explosive, D is the detonation velocity, and K is the adiabatic expansion coefficient of the chemical reaction product gases at the CJ state. Because the detonation velocity and the adiabatic expansion coefficient both increase linearly with the initial density, eq 1 implies that P_{CJ} is proportional to the initial density squared. Measurements of P_{CJ} for various explosives have shown that P_{CJ} is indeed proportional to the square of the initial density. Therefore, to develop more powerful explosives, energetic molecules with very high densities must be identified.

The CJ pressure of an explosive can be calculated to within experimental measurement accuracy by a thermodynamic equilibrium computer code, such as the TIGER code (*3*), or, for explosives containing only C, H, O, and N atoms, by the empirical formula of Kamlet et al. (*10*). These methods require only the molecular formula, the heat for formation, and the initial density of the explosive as input data for a CJ detonation calculation. Hardesty and Kennedy (*9*) recently developed an approximate method of estimating the effective specific energy of an explosive in metal acceleration applications that requires this same input data. The group additivity approach to heat of formation estimation (*1*, *16*) is usually accurate to within ±2 kcal/mol; and, since explosives release 200–500 kcal/mol of energy when detonated, this approach may be confidently used in detonation calculations for hypothetical explosive molecules. Reliable detonation calculations thus require only an accurate method of estimating densities of explosives. This paper presents density estimations for known explosives and related compounds obtained using the group additivity approach.

The prediction of the density of a solid or liquid explosive with no knowledge of its physical properties is difficult; no general method to predict the density of complex organic molecules exists. Three general approaches to density prediction were reviewed: potential function, the theory of close packing for solids, and group additivity. The potential function approach is attractive because it evolves from first principles, and some recent progress (*15*) has been made in its application to large organic molecules. However, as shown by Lee et al. (*14*), the

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Table I. Density Estimations for 25 Known Solid Aromatic Explosives Containing NO_2, OH, CH_3, and NH_2 Groups[a]

explosive	mol wt	measd density, g/cm^3	groups present	calcd molar volume, cm^3/mol	calcd density, g/cm^3	% error
o-dinitrobenzene	168.11	1.565	4(Ca-H) + 2(Ca-NO_2)	106.90	1.572	0.447
m-dinitrobenzene	168.11	1.575	4(Ca-H) + 2(Ca-NO_2)	106.90	1.572	0.190
p-dinitrobenzene	168.11	1.625	4(Ca-H) + 2(Ca-NO_2)	106.90	1.572	3.262
1,3,5-trinitrobenzene	213.11	1.688	3(Ca-H) + 3(Ca-NO_2)	124.72	1.709	1.244
1,2,4-trinitrobenzene	213.11	1.73	3(Ca-H) + 3(Ca-NO_2)	124.72	1.709	1.214
hexanitrobenzene	348.10	1.988	6(Ca-NO_2)	178.18	1.954	1.710
3,5-dinitrophenol	184.11	1.702	3(Ca-H) + 2(Ca-NO_2) + (Ca-OH)	111.04	1.658	2.585
2,3-dinitrophenol	184.11	1.681	3(Ca-H) + 2(Ca-NO_2) + (Ca-OH)	111.04	1.658	1.368
2,4-dinitrophenol	184.11	1.683	3(Ca-H) + 2(Ca-NO_2) + (Ca-OH)	111.04	1.658	1.485
3,4-dinitrophenol	184.11	1.672	3(Ca-H) + 2(Ca-NO_2) + (Ca-OH)	111.04	1.658	0.837
picric acid	229.10	1.763	2(Ca-H) + 3(Ca-NO_2) + (Ca-OH)	128.86	1.778	0.851
styphnic acid	245.10	1.829	(Ca-H) + 3(Ca-NO_2) + 2(Ca-OH)	133.01	1.843	0.765
2,4-dinitrotoluene	182.14	1.521	3(Ca-H) + 2(Ca-NO_2) + (Ca-CH_3)	120.99	1.505	1.052
2,4,6-trinitrotoluene (TNT)	227.13	1.654	2(Ca-H) + 3(Ca-NO_2) + (Ca-CH_3)	138.81	1.636	1.088
2,3,4-trinitrotoluene	227.13	1.620	2(Ca-H) + 3(Ca-NO_2) + (Ca-CH_3)	138.81	1.636	0.988
2,4,5-trinitrotoluene	227.13	1.620	2(Ca-H) + 3(Ca-NO_2) + (Ca-CH_3)	138.81	1.636	0.988
2,4,6-trinitro-*m*-xylene	241.16	1.604	(Ca-H) + 3(Ca-NO_2) + 2(Ca-CH_3)	152.89	1.577	1.683
2,3,6-trinitro-*p*-xylene	241.16	1.590	(Ca-H) + 3(Ca-NO_2) + 2(Ca-CH_3)	152.89	1.577	0.818
1,3,5-trimethyl-2,4,6-trinitrobenzene	255.19	1.48	3(Ca-NO_2) + 3(Ca-CH_3)	166.98	1.528	3.243
2,4-dinitroaniline	183.12	1.615	3(Ca-H) + 2(Ca-NO_2) + (Ca-NH_2)	110.69	1.654	2.415
2,4,6-trinitroaniline	228.12	1.762	2(Ca-H) + 3(Ca-NO_2) + (Ca-NH_2)	128.51	1.775	0.744
2,3,4,6-tetranitroaniline	273.12	1.867	(Ca-H) + 4(Ca-NO_2) + (Ca-NH_2)	146.33	1.867	0.000
1,3-diamino-2,4,6-trinitrobenzene	243.14	1.837	(Ca-H) + 3(Ca-NO_2) + 2(Ca-NH_2)	132.30	1.838	0.054
1,3,5-triamino-2,4,6-trinitrobenzene	258.15	1.938	3(Ca-NO_2) + 3(Ca-NH_2)	136.08	1.897	2.113
3-methyl-2,4,6-trinitrophenol	243.13	1.69	(Ca-H) + 3(Ca-NO_2) + (Ca-OH) + (Ca-CH_3)	142.41	1.707	1.006

[a] Group values used in calculations: -Ca-NO_2 = 29.697 cm^3/mol; -Ca-H = 11.876 cm^3/mol, -Ca-OH = 16.019 cm^3/mol, -Ca-CH_3 = 25.963 cm^3/mol, -Ca-NH_2 = 15.663 cm^3/mol. Ca designates an aromatic carbon atom. Average density = 1.692 g/cm^3, average % error = 1.286%, number of compounds with 0 to 1% error = 11, number of compounds with 1 to 2% error = 9, number of compounds with 2 to 3.3% error = 5.

Table II. Calculated Group Molar Volumes for Aliphatic Compounds

group configuration	letter designation	molar volume, cm^3/mol
C-C, H_3	a	30.68
C-C, H_2, NO_2	b	42.61
C-C_2, H_2	c	15.69
C-C_2, H, NO_2	d	29.16
C-C, $(NO_2)_3$	e	74.86
C-C, H, $(NO_2)_2$	f	59.12
C-C_2, $(NO_2)_2$	g	40.87
C-C, O, = O	h	21.88
C-C, H_2, O	i	16.84
C-C, H_2, OH	j	28.00
C-C, H_2, F	k	31.22
C-C_2, H, OH	l	15.12
C-C_3, OH	m	1.94
C-C, =O, OH	n	23.01
C-C, H, =C	o	12.11
C-C, H_2, ONO_2 (PETN)	p	34.41
C-H_2, =C	q	20.05
C-C, F_2, NO_2	r	59.92
C-C_2, F_2	s	25.63
C-C, F_3	t	46.28
C-C, F, $(NO_2)_2$	u	65.83
C-H_2, O_2	v	33.32
C-C, H_2, ONO_2 (NG)	w	51.21
C-C_4	x	41.49
C-C_3, NO_2	y	71.23
C-C_2, H, ONO_2	z	40.39

potential function approach is mainly concerned with minimizing the potential energies for an arbitrary set of potential functions and then calculating the resulting interaction energies. Density estimates obtained as a secondary feature of the approach are sometimes inaccurate (*14*) and development of an accurate potential function approach to density prediction would be very expensive and time consuming.

For solid organic molecules, a great amount of crystallographic data has been generated and summarized by Kitagorodskii (*11*, *12*). A theory of close packing has been developed to explain the measured densities of solid crystals. However, this crude theory relies on experimentally measured packing coefficients for each molecule. Although several groups are working on the problem (*2*), no theoretical explanation of the measured packing coefficients exists. Therefore the crystallographic close packing approach is not sufficiently developed to use as a tool for predicting densities of solid explosives.

The group additivity approach to density prediction was used by Exner (*6*) to estimate the densities of 870 organic liquids. The densities of very simple liquids were determined to within a standard deviation of 0.003 g/cm^3. For liquids comparable in complexity to most liquid explosives, the densities were determined to within a standard deviation of 0.008 g/cm^3. Exner concluded that the group additivity approach is invalid only for liquids with extremely branched chains or directly bonded functional groups.

No corresponding study of solid compounds by the group additivity approach has been previously reported. The greater degree of internal ordering and the possible existence of more than one stable polymorphic form make density prediction more difficult in solids. However, because group additivity works well for liquids and because the other two approaches cannot be easily developed, the group additivity approach was selected for density prediction in both solid and liquid explosives.

The resulting density estimations for 188 known explosives and related compounds are reported in the next section of this paper. The conclusions and recommendations for future work follow.

Results

Because the main objective of this research effort was to determine the general usefulness of the group additivity approach in predicting explosive densities, an effort was made to calculate

Table III. Density Estimations for Aliphatic Compounds Containing NO_2, OH, F, CO_2H, and ONO_2 Groups[a]

compound	mol wt	measd density, g/cm^3	groups present[b]	calcd molar volume	calcd density, g/cm^3	% error
$CH_3CH_2NO_2$	75.07	1.045	a + b	73.29	1.024	1.98
$CH_3(CH_2)_2NO_2$	89.09	1.008	a + b + c	88.98	1.001	0.67
$CH_3(CH_2)_3NO_2$	103.12	0.971	a + b + 2c	104.67	0.9852	1.46
$CH_3(CH_2)_4NO_2$	131.18	0.949	a + b + 4c	136.05	0.9642	1.60
$CH_3CH(NO_2)CH_3$	89.09	0.988	2a + d	90.52	0.9842	0.38
$O_2NCH_2CH_2NO_2$	120.06	1.46	2b	85.22	1.409	3.49
$(O_2N)_3CC(NO_2)_3$	300.05	1.998	2e	149.72	2.004	0.30
$CH_3CH(NO_2)CH_2CH_3$	103.12	0.985	2a + c + d	106.21	0.9709	1.43
$CH_3CH(NO_2)_2$	120.06	1.350	a + f	89.80	1.337	0.97
$CH_3CH_2CH(NO_2)_2$	134.09	1.261	a + c + f	105.49	1.271	0.80
$O_2NCH_2CH_2CH_2NO_2$	134.09	1.353	2b + c	100.91	1.329	1.77
$CH_3C(NO_2)_2CH_3$	134.09	1.30	2a + g	102.23	1.312	0.90
$O_2NCH_2C(=O)OCH_2CH_3$	133.10	1.1953	a + b + h + i	112.01	1.1883	0.59
$HOCH_2CH_2NO_2$	91.07	1.270	b + j	70.61	1.290	1.56
CH_3CH_2OH	46.07	0.7893	a + j	58.68	0.7853	0.53
$CH_3(CH_2)_2OH$	60.10	0.8035	a + c + j	74.37	0.8081	0.58
$CH_3CH(OH)CH_3$	60.10	0.7855	2a + l	76.48	0.7858	0.04
$CH_3CH(NO_2)CH_2OH$	105.09	1.1841	a + d + j	87.84	1.1964	1.04
$(CH_3)_3COH$	74.12	0.7887	3a + m	93.98	0.7887	
$CH_3CH_2CH_2CH_2OH$	74.12	0.8098	a + 2c + j	90.06	0.8230	1.63
$CH_3CH(OH)CH_2CH_3$	74.12	0.8080	2a + c + l	92.17	0.8042	0.47
$C_2H_5CH(NO_2)CH_2OH$	119.12	1.1332	a + c + d + j	103.53	1.1506	1.53
$CH_3(CH_2)_4OH$	88.15	0.8144	a + 3c + j	105.75	0.8336	2.35
$CH_3CH(OH)(CH_2)_2CH_3$	88.15	0.8103	2a + 2c + l	107.86	0.8173	0.86
$C_2H_5CH(OH)C_2H_5$	88.15	0.8212	2a + 2c + l	107.86	0.8173	0.48
HO_2CCO_2H	90.03	1.900	2n	46.02	1.956	2.96
$HO_2CCH_2CO_2H$	104.06	1.619	c + 2n	61.71	1.686	4.16
$HO_2(CH_2)_2CO_2H$	118.09	1.572	2c + 2n	77.40	1.526	2.94
$HO_2C(CH_2)_3CO_2H$	132.12	1.424	3c + 2n	93.09	1.419	0.33
$HO_2C(CH_2)_4CO_2H$	146.14	1.360	4c + 2n	108.78	1.343	1.21
$HO_2C(CH_2)_8CO_2H$	202.25	1.2705	8c + 2n	171.54	1.179	7.20
$C_2H_5C(=O)OCH_2C(=O)OC_2H_5$	160.17	1.0551	2a + c + 2h + 2i	154.49	1.0368	1.74
$C_2H_5CO_2(CH_2)_2CO_2C_2H_5$	174.20	1.0402	2(a + c + h + i)	170.18	1.0236	1.59
$C_2H_5CO_2(CH_2)_3CO_2C_2H_5$	188.22	1.0220	2a + 3c + 2h + 2i	185.87	1.0126	0.92
$C_2H_5CO_2(CH_2)_4CO_2C_2H_5$	202.25	1.0076	2(a + 2c + h + i)	201.56	1.0034	0.41
$C(NO_2)_3CH_2CO_2CO_2CH_2C(NO_2)_3$	416.12		2(e + h + i)	227.16	1.8318	
$C(NO_2)_3CH_2CO_2CH_2CO_2CH_2C(NO_2)_3$	430.15	1.75	c + 2(e + h + i)	242.85	1.7713	1.21
$C(NO_2)_3CH_2CO_2(CH_2)_2CO_2CH_2C(NO_2)_3$	444.18		2(c + e + h + i)	258.54	1.718	
$C(NO_2)_3CH_2CO_2(CH_2)_3CO_2CH_2C(NO_2)_3$	458.21	1.67	3c + 2(e + h + i)	274.23	1.6709	0.05
$C(NO_2)_3CH_2CO_2(CH_2)_4CO_2CH_2C(NO_2)_3$	472.23	1.64	4c + 2(e + h + i)	289.92	1.6288	0.68
$C(NO_2)_3CH_2CO_2(CH_2)_5CO_2CH_2C(NO_2)_3$	486.26	1.63	5c + 2(e + h + i)	305.61	1.5911	2.39
$C(NO_2)_3CH_2CO_2(CH_2)_6CO_2CH_2C(NO_2)_3$	500.29	1.59	6c + 2(e + h + i)	321.30	1.5571	2.07
$C(NO_2)_3CH_2CO_2(CH_2)_7CO_2CH_2C(NO_2)_3$	514.31	1.475	7c + 2(e + h + i)	336.99	1.5262	3.47
$C(NO_2)_3CH_2CO_2(CH_2)_8CO_2CH_2C(NO_2)_3$	528.34	1.45	8c + 2(e + h + i)	352.68	1.498	3.32
$CH_3C(NO_2)_2CH_2CO_2CH=CHCO_2CH_2C(NO_2)_2CH_3$	380.22	1.60	2(a + g + h + i + o)	244.76	1.553	2.91
$HO_2CCH=CHCO_2H$	116.07	1.635	2(n + o)	70.24	1.652	1.04
$C_3H_7CO_2CH=CHCO_2C_3H_7$	200.23	1.0129	2(a + c + h + i + o)	194.40	1.0330	1.69
$C(NO_2)_3(CH_2)_2CO_2CH_2C(NO_2)_2CH_3$	355.17	1.68	a + 2c + e + g + h + i	216.51	1.6404	2.36
$C(NO_2)_3(CH_2)_2CO_2(CH_2)_2CO_2(CH_2)_2C(NO_2)_3$	472.23	1.63	2(2c + e + h + i)	289.92	1.6288	0.07
$C_3H_7CO_2(CH_2)_2CO_2C_3H_7$	202.25	1.002	2(a + 2c + h + i)	201.56	1.0034	0.14

$CH_3C(NO_2)_2CH_2CO_2(CH_2)_2CO_2CH_2C(NO_2)_2CH_3$	382.24	1.51	2(a + c + g + h + i)	251.92	1.5173	0.48
$CH_3CH(NO_2)_2CH_2CO_2CH{=}CH_2$	204.14	1.47	a + g + h + i + o + q	142.43	1.4333	2.50
$C_2H_5CO_2(CH_2)_2C(NO_2)_2CH_3$	220.18	1.28	2a + 2c + g + h + i	172.33	1.2777	0.18
$C_2H_5CO_2C_3H_7$	116.16	0.8785	2a + 2c + h + i	131.46	0.8836	0.58
$C(NO_2)_3(CH_2)_2CO_2CH_2C(NO_2)_3$	386.14	{1.783 1.767}	2c + 2e + h + i	219.82	1.7566	{1.48 0.59}
$CF_2NO_2CF_2NO_2$	192.02	1.6024	2r	119.84	1.6023	
C_3H_7F	62.09	0.7956	a + c + k	77.59	0.8002	0.58
$FCH_2CH_2CH_2F$	80.08	1.0057	c + 2k	78.13	1.0250	1.91
$CH_3CF_2CH_3$	80.08	0.9205	2a + s	86.99	0.9206	
$CF_3CH_2CH_2NO_2$	143.06	1.4205	b + c + t	104.59	1.3678	3.70
$CF_3CH_2NO_2$	129.04	1.3914	b + t	88.89	1.4517	4.33
$CF(NO_2)_2CH_2OCH_2OCH_2CF(NO_2)_2$	320.12	1.607	2(i + u) + v	198.66	1.611	0.27
$(PET)N(CH_2ONO_2)_4C$	316.14	1.77	4p + x	179.13	1.7649	0.29
$CH_3CH_2ONO_2$	91.07	1.100	a + w	81.89	1.1121	1.10
$O_2NOCH_2CH_2ONO_2$	152.06	1.48	2w	102.42	1.4847	0.32
$CH_3C(CH_2ONO_2)_3$	255.14	1.47	a + 3p + x	175.40	1.4546	1.05
$HOCH_2C(CH_2ONO_2)_3$	271.14	1.54	j + 3p + x	172.72	1.5698	1.94
$O_2NC(CH_2ONO_2)_3$	286.11	1.64	3p + y	174.46	1.64	
$NGO_2NOCH_2CH(ONO_2)CH_2ONO_2$	227.09	1.596	2w + z	142.81	1.5902	0.37
$O_2NOCH_2(CHONO_2)_4CH_2ONO_2$	452.15	1.73	2(w + 2z)	263.98	1.7128	0.99
$O_2NOCH_2CH_2CH(ONO_2)CH_2ONO_2$	241.11	1.52	c + 2w + z	158.50	1.5212	0.08
$O_2NOCH_2CH_2OCH_2CH_2ONO_2$	196.12	1.38	2(i + w)	136.10	1.441	4.42
$O_2NOCH_2CH_2OCH_2OCH_2CH_2ONO_2$	226.14	1.33	2i + v + 2w	169.42	1.335	0.36
$O_2NOCH_2CH(ONO_2)CH_2CO_2CH(ONO_2)CH_3$	299.15	1.47	a + h + i + w + 2z	201.39	1.4854	1.05
$(O_2NOCH_2)_3CCH_2OCH_2C(CH_2ONO_2)_3$	524.26	1.63	2(i + 3p + x)	323.12	1.6225	0.46
$(O_2NOCH_2)_3CCH_2OCH_2C(CH_2ONO_2)_2CH_2OCH_2C(CH_2ONO_2)_3$	732.39	1.58	4i + 8p + 3x	467.11	1.5679	0.76
FCH_2CH_2OH	64.06	1.104	j + k	59.22	1.082	1.99
$CH_3CH_2CH(NO_2)CH_2CH_3$	117.15	0.957	2a + 2c + d	121.90	0.9610	0.42
$(CH_2ONO_2)_3CC(CH_2ONO_2)_3$	480.22	1.63	6p + 2x	289.44	1.659	1.79
$O_2NOCH_2CH(OH)CH_2ONO_2$	182.10	1.523	l + 2w	117.54	1.549	1.72

[a] Average density (75 compounds) = 1.3153, average % error (75 compounds) = 1.509%, number of compounds with 0 to 1% error = 35, number of compounds with 1 to 2% error = 24, number of compounds with 2 to 3% error = 8, number of compounds with 3 to 4% error = 4, number of compounds with 4 to 5% error = 3, number of compounds with >5% error = 1. [b] See Table II for definitions.

group values and predict densities for the maximum possible number of explosives and related compounds. For group additivity to be a worthwhile tool in predicting densities of new explosives, it must be applicable to all types of organic explosives: aromatic, aliphatic, alicyclic, and heterocyclic. Therefore density data on these types of compounds were collected from several handbooks (*5*, *7*, *8*, *13*, *17*). In most cases, density data found in two or more sources were in reasonable agreement; but for some compounds, two conflicting density values or only one value from an older, less reliable source was obtained. Thus some of the apparent discrepancies between predicted and measured may represent flaws in certain measured data rather than faults in the predictive scheme.

When the available density data for a series of explosives were assembled, the groups present in each compound were identified and a linear equation was written in terms of molar volume for each compound. A simple computer program was used to calculate the group molar volume contributions that produced the minimum total absolute error in molar volume for that particular set of compounds. Most of the calculated group values are based on data from 10 to 20 compounds and are considered to be reliable, but some of the calculated values for the less common groups are based on only two or three densities and thus are not as reliable. In this first-generation group additivity approach, only one value of the molar volume is assigned to each group, regardless of where it appears in the molecule. No second-order effects, such as nearest-neighbor interactions, phase changes, and crystalline structure changes, are considered when calculating these group values. A discussion of the possibility of including second-order effects in a more sophisticated group additivity approach, similar to the detailed models developed by Benson et al. (*1*) for the estimation of various thermochemical properties, is presented in the last section of this paper.

The first explosives to which the group additivity approach was applied are 25 solid aromatic compounds containing NO_2, OH, CH_3, and NH_2 groups bonded directly to the benzene ring. Only five group values (C_a-H, C_a-NO_2, C_a-OH, C_a-CH_3, and C_a-NH_2, where C_a designates an aromatic carbon atom) are required to describe these compounds. The group molar volumes that give the best overall agreement and the resulting density estimations are shown in Table I. The average error in Table I is 1.29%, which represents 0.022 g/cm^3 based on an average density of 1.692 g/cm^3. The estimated density is within 1% of the reported density for 11 compounds, within 1-2% for 9 compounds, and within 2-3.3% for the other 5 compounds.

The use of only one molar volume for each group does not allow for density differences between isomers. For example, in terms of formulating high-density molecules, it appears to be much more favorable to have nitro groups para to each other rather than ortho or meta. This explains the significantly higher densities of *p*-dinitrobenzene and 1,2,4-trinitrobenzene relative to *m*-dinitrobenzene and 1,3,5-trinitrobenzene, respectively. There also appears to be a smaller advantage in placing nitro groups meta rather than ortho to reduce steric hindrance. Quantifying such effects for all possible nearest-neighbor interactions would result in a slightly improved overall agreement but would greatly increase the number of group values to be determined. The good overall agreement between measured densities and those calculated by using one molar volume per group led to the use of this first generation group additivity technique in predicting densities of explosives bound in other configurations.

Table IV. Calculated Group Molar Volumes for Various Nitrogen Compounds

group configuration	letter designation	molar volume, cm^3/mol
C-C, H_2, NH_2	α	34.42
C-C_2, H, NH_2	β	22.49
C-C, H_2, NH	γ	20.64
C-C_2, H, NH	δ	8.42
C-H_3, NH	ϵ	32.87
C-C, H_2, N	η	16.09
C-H_3, N	θ	31.00
C-C, H_2, N-NO_2	κ	25.57
$[\text{C-C}, H_2, \text{N-}NO_2]_c$	cκ	26.80
C-C_2, H, N-NO_2	λ	9.70
C-H_3, N-NO_2	ξ	38.32
$[\text{C-}H_2, \text{O}, \text{N-}NO_2]_c$	σ	28.02
C-O_4	τ	28.45
C-H, O_3	ψ	26.63
C-C, O, F_2	χ	26.78
C-C_3, H	Ψ	2.96
$(\text{C-}C_2, H_2)_c$	ca	18.38
$[\text{C-}H_2, (\text{N-}NO_2)_2]_c$[a]	cb	41.60
$(\text{C-}C_2, H_2)_{c=8}$[b]		16.80
$[\text{C-}H_2, (\text{N-}NO_2)_2]_{c=8}$		40.02
$(\text{C-C}, H_2, \text{O})_c$	cc	21.75
$(\text{C-C}, \text{H}, =\text{C})_c$	cd	15.12
$(\text{C-H}, \text{O}, =\text{C})_c$	ce	20.66
$(\text{C-H}, =\text{C}, \text{NH})_c$	cf	19.81
$(\text{N-C}, \text{H}, \text{NH})_c$	cg	11.45
$(\text{C-H}, =\text{C}, \text{N})_c + (\text{C-H}, \text{N}, =\text{N})_c$	ch	46.27
$(\text{C-C}, H_2, \text{NH})_c$	ci	22.35
$(\text{C-}C_2, =\text{O})_c$	cj	13.44
$(\text{C-}C_2, \text{H}, NO_2)_c$	ck	31.58
$(\text{C-}C_2, \text{H}, \text{OH})_c$	cl	12.17
$(\text{C-}C_4)_c$	cm	24.67
$(\text{C-}O_4)_c$	cn	11.63
$(\text{C-}NO_2, \text{O}, =\text{C})_c$	co	33.53
$(\text{C-C}, \text{F}, =\text{C})_c$	cp	20.21
$(\text{C-C}, \text{H}, \text{O}, NO_2)_c$	cq	36.04
$[\text{C-}C_2, (NO_2)_2]_c$	cr	43.56
$[\text{C-}(\text{N-}NO_2)_2, =\text{O}]_c$	cs	36.66
$[\text{C-C}, \text{H}, (\text{N-}NO_2)_2]_c$	ct	42.68
$[\text{C-C}, \text{F}, (\text{N-}NO_2)_2]_c$	cu	47.77
$[\text{C-}F_2, (\text{N-}NO_2)_2]_c$	cv	51.78
$(\text{C-}C_2, =\text{N})_c + (\text{N-O}, =\text{C})_c$	cw	15.92
$(\text{C-H}, \text{C}, =\text{N})_c + (\text{N-O}, =\text{C})_c$	cx	28.28
$(\text{C-C}, \text{N}, =\text{N})_c + (\text{N-C}, =\text{C})_c$	cy	11.82
$(\text{C-C}, \text{O}, =\text{N})_c + (\text{N-O}, =\text{C})_c$	cz	20.38
C_a-N(H, C)[c]		20.38
C_a-N(C, C)		8.54
C_a-N(C, NO_2)		21.66

[a] Subscript "c" denotes a group from a cyclic compound containing a five- or six-membered ring. [b] Subscript "c=8" denotes a group from an eight-membered ring. [c] As in Table I, C_a designates an aromatic carbon atom.

The second major series of explosives and related compounds consists of 80 aliphatic compounds containing NO_2, OH, F, CO_2H, and ONO_2 groups. Table II lists the calculated molar volumes for the 26 group configurations found in these compounds. Most of the group values are determined by comparing densities of 10-20 compounds containing that group, but seven of the group values (denoted by the letters f, m, q, r, s, t, and y in Table II) are determined from density data on only two or three compounds and are considered to be less reliable. In the case of C-C, H_2, and ONO_2 groups, two molar volumes are used. One value is used for nitrate esters similar to pentaerythritol tetranitrate (PETN) in which three or four C-C, H_2, and ONO_2 groups are bonded to a central carbon atom; another molar volume is used for nitrate esters like nitroglycerine (NG) that have C-C, H_2, and ONO_2 groups bonded to separate carbon atoms.

The resulting density estimations of these 80 aliphatic compounds are shown in Table III. Direct comparisons between the measured and calculated densities can be made for 74 of the 80 compounds. The average error is 1.51%, which represents 0.0199 g/cm^3 based on the average density of 1.3153 g/cm^3. Of the estimated densities, 47% are within 1% of the reported densities and another 32% are within 1 to 2% of the reported densities. Large errors occur for compounds with bulky or highly polar groups bonded in close proximity, such as oxalic acid and malonic acid. In the previously mentioned statistical study of density estimation by group additivity in liquids, Exner (*6*) concluded that the approach is least accurate for highly branched chains containing several polar groups. This problem appears to be a real limitation of the group additivity approach in its present form, but it exists for only a small number of potential explosives. Second-order effects must definitely be considered to improve the density estimations for these explosives.

Many other existing and potential explosives are derivatives of amino, alicyclic, and heterocyclic compounds. Table IV lists the calculated molar volumes for the 47 group configurations required to describe the 83 amines, nitramines, and cyclic compounds whose density estimations are tabulated in Table V. Because nearly all the cyclic compounds considered contain a five- or six-membered ring, the group values with a subscript c in Table IV are derived from the available density data on alicyclic and heterocyclic compounds containing five- or six-membered rings. In general, the cyclic group molar volumes are a few cubic centimeters per mole larger than those of the corresponding aliphatic groups. The molar volumes of two groups found in eight-membered rings (labeled with the subscript c = 8 in Table IV) had to be determined to estimate the density of HMX relative to RDX. The molar volume of the group $[C-H_2, (N-NO_2)_2]_{c=8}$ found in HMX was calculated by taking the value for the corresponding group in RDX, $[C-H_2, (N-NO_2)_2]_c$, and subtracting the difference between the groups $(C-C_2, H_2)_{c=8}$, which was determined by the density of cyclooctane, and $(C-C_2, H_2)_c$ for five- and six-membered rings. This simple difference between a six- and an eight-membered ring explains most of the difference in the densities of RDX and HMX. The calculated densities differ by 0.07 g/cm^3, the measured densities are 0.094 g/cm^3 apart.

Direct comparisons of the measured and estimated densities can be made for 73 of the 83 compounds listed in Table V. The average error is 1.681%, which represents 0.0174 g/cm^3 based on an average density of 1.0355 g/cm^3. Of the estimated densities, 33% are within 1% of the reported values, 33% are within 1 to 2%, and another 25% are within 2 to 3%. This overall agreement is quite reasonable when compared with the results in Table I and III and when the diverse nature of the compounds in Table V is considered.

Undoubtedly there are other explosives and related compounds whose densities have been measured, but the 188 compounds in Tables I, III, and V represent those obtained during a fairly extensive review of the open literature. The group molar volumes listed in Tables II and IV should cover most other existing compounds. The overall results of the density estimations by this first-generation group additivity approach for the 173 compounds whose estimated and measured densities can be compared are summarized in Table VI. Of the estimated densities, 73.4% are within 2% of the measured densities, with another 16.8% within 2 to 3%. These results and the conclusions that can be drawn from them are discussed more fully in the next section.

Conclusions and Recommendations

The main conclusion regarding the applicability of the group additivity approach to density estimation is that the results are very promising. A total of 173 explosives and related compounds of very diverse natures were considered in a first-generation group additivity approach, and 40.5% of the estimated densities were within 1% of the measured densities, 33.0% were within 1 to 2%, 16.8% were within 2 to 3%, 5.2% were within 3 to 4%, and 4.6% were more than 4% different from the reported densities. A 3% error in the estimated density of an explosive that has an actual density of 2.0 g/cm^3 and a CJ pressure of 400 kbar would cause an error of approximately 24 kbar in the estimated CJ pressure, because pressure varies as the square of the density. This 6% error is within the experimental uncertainties of various methods of measuring the CJ pressure (*4*). Therefore, an error of this magnitude would not affect a decision about the usefulness of a new explosive molecule based on a CJ pressure calculation. Of the densities estimated in this study, 90.2% were within 3% of the measured density and thus would yield realistic estimates of the CJ pressure. The average absolute error in density was 0.019 08 g/cm^3 in Tables I, III, and V and may represent a better indication of the accuracy of the group additivity approach than the percent errors. The absolute error in density exceeded 0.05 g/cm^3 for only 14 of the 173 compounds (8.09%). Therefore 92% of the estimated densities could be used with confidence in CJ calculations.

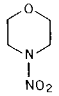
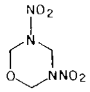
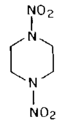
As mentioned previously, the largest errors occurred for compounds with several bulky, highly polar groups in close proximity and for compounds that contain groups whose calculated molar volumes were based on density data for only two or three compounds. As more density data become available for a certain group configuration, the molar volume can be determined more accurately and the overall agreement between measured and estimated densities of compounds containing that group improved. Therefore, it is very important to obtain as much density information as possible for a series of related compounds before deriving the group values.

From the results of Exner (*6*) and of this study, it can be concluded that the group additivity approach estimates densities of liquids very accurately, except in a few cases of very highly branched, polar molecules. Table VII shows the breakdown of the density estimation accuracies according to the physical state of the compound at room temperature. The standard deviation in the density estimations for the 102 liquids in Tables III and V is 0.0194 g/cm^3. This standard deviation compares favorably with the standard deviation of 0.008 g/cm^3 obtained by Exner (*6*) when the diverse nature and molecular complexities of the 102 liquids in the current study are considered. Group additivity is therefore a useful density estimation tool for the many liquid explosives that are known and those that may be synthesized. Inclusion of second-order effects, such as correction factors for nearest-neighbor interactions, would reduce the errors in density for the highly branched polar molecules.

The group additivity approach also worked well for solid explosives when the group values were determined from data on many similar compounds, such as the aromatic compounds in Table I. Slight differences in the crystalline packing geometries of these compounds were effectively averaged over as the group molar volumes were determined. Table VII shows that the average percentage error for the 71 solid compounds investigated is the same as that for the 102 liquids, but there are more solids with relatively large absolute errors. Of the 30 compounds with absolute density errors of more than 0.03 g/cm^3, 22 are solids. Taking into account the greater densities and geometrical complexities of the solid compounds, we found that the overall agreement of this first-generation group additivity approach with reported solid densities is quite good. In groups of compounds that are not as similar as the aromatic explosives and in single compounds like HMX that have several stable polymorphic forms, the difference in crystal geometries could have significant effects on the actual density. The first-generation group additivity approach used in this study cannot predict these density changes. However, inclusion of second-order corrections for the various possible crystal configurations may allow group additivity to successfully predict different densities for various polymorphs of a solid explosive.

On the basis of the accuracy of the group additivity approach in predicting densities of liquid and solid explosives, and on the need for a reliable approach to density estimation for hypothetical explosive molecules, the group additivity approach will be

Table V. Density Estimations for Amines, Nitramines, and Various Cyclic Compounds[a]

compound	mol wt	measd density, g/cm³	groups present[b]	calcd molar volume	calcd density, g/cm³	% error
$H_2NCH_2CH_2NH_2$	60.11	0.8995	2α	68.84	0.8732	2.93
$CH_3CH(NH_2)CH_2NH_2$	74.13	0.8584	$a + \alpha + \beta$	87.59	0.8463	1.41
$NH_2CH_2CH_2CH_2NH_2$	74.13	0.884	$c + 2\alpha$	84.53	0.8770	0.80
$H_2N(CH_2)_4NH_2$	88.15	0.877	$2c + 2\alpha$	100.22	0.8796	0.29
$CH_3(CH_2)_3NH_2$	73.14	0.7414	$a + 2c + \alpha$	96.48	0.7581	2.25
$CH_3CH(NH_2)CH_2CH_3$	73.14	0.724	$2a + c + \beta$	99.54	0.7348	1.49
$CH_3(CH_2)_3NHC_2H_5$	101.19	0.7398	$2a + 2c + 2\gamma$	134.02	0.7550	2.06
$CH_3CH_2CH(CH_3)NHC_2H_5$	101.19	0.7396	$3a + c + \gamma + \delta$	136.79	0.7397	0.02
$(C_2H_5)_2NH$	73.14	0.7056	$2a + 2\gamma$	102.64	0.7126	0.99
$(CH_3)_2NH$	45.09	0.6804	2ϵ	65.74	0.6859	0.81
$(C_5H_{11})_2NH$	157.30	0.7771	$2a + 6c + 2\gamma$	196.78	0.7994	2.87
$(C_4H_9)_2NH$	129.25	0.7670	$2a + 4c + 2\gamma$	165.40	0.7814	1.88
$(C_3H_7)_2NH$	101.19	0.7400	$2a + 2c + 2\gamma$	134.02	0.7550	2.03
$[(CH_3)_2CH]_2NH$	101.19	0.7169	$4a + 2\delta$	139.56	0.7251	1.14
$H_2N(CH_2)_2NH(CH_2)_2OH$	104.15	1.0254	$j + \alpha + 2\gamma$	103.70	1.0043	2.05
$(HOCH_2CH_2)_2NH$	105.14	1.09664	$2j + 2\gamma$	97.28	1.0808	1.44
$HO(CH_2)_2NHCH_2CH(OH)C_2H_5$	133.19	1.0310	$a + c + j + l + 2\gamma$	130.77	1.0185	1.21
$HO(CH_2)_2NH(CH_2)_2CH(OH)CH_3$	133.19	1.0331	$a + c + j + l + 2\gamma$	130.77	1.0185	1.41
$c\text{-}C_6H_{11}NH\text{-}c\text{-}C_6H_{11}$	181.33	0.9123	$10ca + 2\delta$	200.64	0.9038	0.94
$CH_3NH(CH_2)_2NHCH_3$	88.15	0.828	$2\gamma + 2\epsilon$	107.02	0.8237	0.52
$(CH_3)_3N$	59.11	0.6356	3θ	93.00	0.6356	
$(C_2H_5)_3N$	101.19	0.7275	$3a + 3\eta$	140.31	0.7212	0.87
$(C_3H_7)_3N$	143.28	0.7558	$3a + 3c + 3\eta$	187.38	0.7646	1.17
$(C_4H_9)_3N$	185.36	0.7771	$3a + 6c + 3\eta$	234.45	0.7906	1.74
$[(CH_3)_2CHCH_2]_3N$	185.36	0.7684	$6a + 3\psi + 3\eta$	241.23	0.7684	
$(C_5H_{11})_3N$	227.44	0.7907	$3a + 9c + 3\eta$	281.52	0.8079	2.18
$(HOCH_2CH_2)_2NC_2H_5$	133.19	1.0135	$a + 2j + 3\eta$	134.95	0.9870	2.62
$(HOCH_2CH_2)_3N$	149.19	1.1242	$3j + 3\eta$	132.27	1.1272	0.33
$(CH_3)_2NNO_2$	90.08	1.109	2ξ	76.64	1.175	5.95
$(C_2H_5)_2NNO_2$	118.14	1.057	$2a + 2\kappa$	112.50	1.050	0.65
$(C_3H_7)_2NNO_2$	146.19	0.995	$2a + 2c + 2\kappa$	143.88	1.016	2.12
$(C_4H_9)_2NNO_2$	174.24	0.962	$2a + 4c + 2\kappa$	175.26	0.9942	3.35
$[(CH_3)_2CH]_2NNO_2$	146.19	1.104	$4a + 2\lambda$	132.42	1.104	
$CH_3N(NO_2)(CH_2)_2N(NO_2)CH_3$	178.15	1.446	$2\xi + 2\kappa$	127.78	1.394	3.58
	132.12	1.363	$2c\kappa + 2cc$	97.10	1.3607	0.17
	178.10	1.824	$2\sigma + 2cb$	97.64	1.824	
	176.13	1.638	$4c\kappa$	107.20	1.643	0.31
cyclopentane	70.14	0.7457	$5ca$	91.90	0.7632	2.35
cyclohexane	84.16	0.77855	$6ca$	110.28	0.7631	1.98
cyclooctane	112.22	0.8349	$8[C\text{-}C_2, H_2]_{c=8}$	134.41	0.8349	
RDX	222.12	1.806	$3cb$	124.80	1.780	1.44
HMX	296.16	1.900	$4[C\text{-}H_2, (N\text{-}NO_2)_2]_{c=8}$	160.08	1.850	2.63

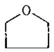
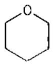
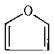
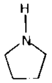
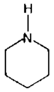
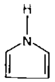
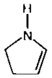
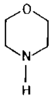
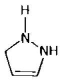
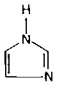
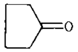
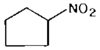
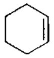
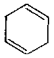
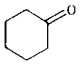
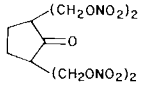
N-propylaniline	135.21	0.9443	a + c + η + 5[Ca–H] + [Ca–N(H, C)]	142.24	0.9506	0.66
N-methylaniline	107.16	0.98912	θ + 5[Ca–H] + [Ca–N(H, C)]	110.78	0.9673	2.20
N-ethylaniline	121.18	0.9625	a + η + 5[Ca–H] + [Ca–N(H, C)]	126.55	0.9576	0.51
N,*N*-diethylaniline	149.24	0.93507	2a + 2η + 5[Ca–H] + [Ca–N(C, C)]	161.48	0.9242	1.16
N,*N*-dipropylaniline	177.29	0.9104	2a + 2c + 2η + 5[Ca–H] + [Ca–N(C, C)]	192.86	0.9193	0.97
N-butylaniline	149.24	0.93226	a + 2c + η + 5[Ca–H] + [Ca–N(H, C)]	157.93	0.9450	1.37
tetryl	287.14	1.73	3[Ca–NO_2] + 2[Ca–H] + θ + [Ca–N(C, NO_2)]	165.12	1.739	0.52
	72.12	0.8892	2ca + 2cc	80.26	0.8986	1.05
	86.14	0.8810	3ca + 2cc	98.64	0.8733	0.88
	68.08	0.9514	2cd + 2ce	35.78	0.9514	
	71.12	0.8520	2ca + 2ci	81.46	0.8731	2.47
	85.15	0.8606	3ca + 2ci	99.84	0.8529	0.90
	67.09	0.9691	2cd + 2cf	69.86	0.9603	0.90
	69.11	0.9097	ca + ci + cf + cd	75.66	0.9134	0.41
	87.12	1.0005	2cc + 2ci	88.20	0.9878	1.27
	70.10	1.0200	ci + cd + cf + cq	68.73	1.0200	
	68.08	1.0303	cf + ch	66.08	1.0303	
	68.13	0.7720	3ca + 2cd	85.38	0.7980	3.36
	66.10	0.8021	ca + 4cd	78.86	0.8382	4.50
	84.19	0.94869	4ca + cj	86.96	0.9681	2.05
	115.13	1.0776	4ca + ck	105.10	1.0954	1.65
	82.15	0.8102	4ca + 2cd	103.76	0.7917	2.28

Table V (*Continued*)

compound	mol wt	measd density, g/cm^3	groups present[b]	calcd molar volume	calcd density, g/cm^3	% error
	80.14	0.8405	2ca + 4cd	97.24	0.8242	1.94
	80.14	0.8471	2ca + 4cd	97.24	0.8242	2.70
	98.14	0.9478	5ca + cj	105.34	0.9316	1.70
c-$C_6H_{11}NO_2$	129.16	1.0610	5ca + ck	123.48	1.0460	1.41
c-$C_6H_{11}OH$	100.16	0.9624	5ca + cl	104.07	0.9624	
	384.22	1.62	2ca + cj + 2cm + 4p	237.17	1.62	
$C(OCH_2CH_3)_4$	192.26	0.9186	τ + 4a + 4i	218.53	0.8798	4.22
$C(OC_3H_7)_4$	248.36	0.897	τ + 4a + 4c + 4i	281.29	0.8829	1.57
$C[OCH_2C(NO_2)_3]_4$	732.22	1.84	τ + 4e + 4i	395.25	1.8525	0.68
$C[OCH_2CF(NO_2)_2]_4$	624.19	1.71	τ + 4i + 4u	359.13	1.738	1.64
$HC[OC_2H_5]_3$	148.20	0.8909	ψ + 3a + 3i	169.19	0.8760	1.67
$HC[OC_3H_7]_3$	190.28	0.8805	ψ + 3a + 3c + 3i	216.26	0.8799	0.07
$HC[OCH_2C(NO_2)_3]_3$	553.18	1.80	ψ + 3e + ei	301.73	1.8334	1.85
$HC[OCH_2CF(NO_2)_2]_3$	472.15	1.76	ψ + 3i + 3u	274.64	1.719	2.32
$H_2C[OC_2H_5]_2$	104.15	0.8319	v + 2a + 2i	128.36	0.8114	2.47
$H_2C(OC_3H_7)_2$	122.12	0.8345	v + 2a + 2c + 2i	159.74	0.8276	0.83
$H_2C[OCH_2C(NO_2)_3]_2$	374.13	1.72	v + 2e + 2i	216.72	1.7263	0.38
$[(NO_2)_3CCH_2]_2NNO_2$	388.15	1.96	2e + 2κ	200.86	1.9324	1.41
$[F(NO_2)_2CCH_2]_2NNO_2$	334.13	1.91	2u + 2κ	182.84	1.8274	4.32

[a] Average density (73 compounds) = 1.0355 g/cm^3, average % error (73 compounds) = 1.681%, number of compounds with 0 to 1% error = 24, number of compounds with 1 to 2% error = 24, number of compounds with 2 to 3% error = 18, number of compounds with 3 to 4% error = 3, number of compounds with 4 to 5% error = 3, number of compounds with >5% error = 1. [b] See Tables II and IV for definitions.

Table VI. Summary of the Accuracy of the Group Additivity Approach to Density Estimation

% error range	no. of compd within this range of density estimation error	% of compd studied within this range
0-1	70	40.46
1-2	57	32.95
2-3	29	16.76
3-4	9	5.20
4-5	6	3.47
>5	2	1.16
total	173	100.00

Average Density (188 compounds) = 1.2517 g/cm^3
Average % Error (173 compounds) = 1.524%
Average Absolute Error in Density = 0.01908 g/cm^3

absolute error range, g/cm^3	no. of compd with this range	% of compd studied within this range
0.00-0.01	58	33.53
0.01-0.02	59	34.10
0.02-0.03	26	15.03
0.03-0.04	10	5.78
0.04-0.05	6	3.47
0.05-0.06	7	4.05
0.06-0.07	5	2.89
0.07-0.08	0	0.00
0.08-0.09	1	0.58
0.09-0.10	1	0.58

Standard Deviation = 0.0254 g/cm^3

extended to include second-order corrections for phase changes, nearest-neighbor interactions, effects of crystal geometry, and other factors. Together with CJ pressure and metal acceleration calculation techniques and a related synthesis program, an expanded group additivity approach will constitute a rapid and relatively inexpensive method for the development of more powerful candidate explosives.

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Table VII. Comparison of the Density Estimation Results for Liquid and Solid Compounds

	liquids (102 compd)	solids (71 compd)
av density, g/cm^3	0.9917	1.6252
av % error	1.529	1.517
av abs error, g/cm^3	0.0153	0.0246
stand dev, g/cm^3	0.0194	0.0322
no. of compd within an abs error range		
0.00-0.01 g/cm^3	39 (38.24%)	19 (26.76%)
0.01-0.02 g/cm^3	41 (40.20%)	18 (25.35%)
0.02-0.03 g/cm^3	14 (13.73%)	12 (16.90%)
0.03-0.04 g/cm^3	3 (2.94%)	7 (9.86%)
0.04-0.05 g/cm^3	0	6 (8.45%)
0.05-0.06 g/cm^3	3 (2.94%)	4 (5.63%)
0.06-0.07 g/cm^3	2 (1.96%)	3 (4.23%)
0.07-0.08 g/cm^3	0	0
0.08-0.09 g/cm^3	0	1 (1.41%)
0.09-0.10 g/cm^3	0	1 (1.41%)

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