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Revision and Extension of a Generally Applicable Group-Additivity Method for the Calculation of the Refractivity and Polarizability of Organic Molecules

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Abstract: In a continuation and extension of an earlier publication, the calculation of the refractivity and polarizability of organic molecules at standard conditions is presented, applying a commonly applicable computer algorithm based on an atom-group additivity method, where the molecules are broken down into their constituting atoms, these again being further characterized by their immediate neighbor atoms. The calculation of their group contributions, carried out by means of a fast Gauss–Seidel fitting calculus, used the experimental data of 5988 molecules from literature. An immediate subsequent ten-fold cross-validation test confirmed the extraordinary accuracy of the prediction of the molar refractivity, indicated by a correlation coefficient R^2 and a cross-validated analog Q^2 of 0.9997, a standard deviation σ of 0.38, a cross-validated analog S of 0.41, and a mean absolute deviation of 0.76%. The high reliability of the predictions has been exemplified with three classes of molecules: ionic liquids, silicon- and boron-containing compounds. The corresponding molecular polarizabilities have been calculated indirectly from the refractivity using the inverse Lorentz-Lorenz relation. In addition, it could be shown that there is a close relationship between the "true" volume and the refractivity of a molecule, revealing an excellent correlation coefficient R^2 of 0.9645 and a mean absolute deviation of 7.53%.

Keywords: group-additivity method; Gauss-Seidel diagonalization; refractivity; polarizability; ionic liquids; silanes; boranes

1. Introduction

In continuation of an earlier paper [1], which used a generally applicable atom-groups additivity method for the prediction of various molecular descriptors including the refractivity and the polarizability of molecules, the present work puts the focus on the latter two descriptors, for which on the one hand an extended number of further experimental refractivity data has been included in the atom-group parameters calculation, and on the other hand a different method for the prediction of the polarizability has been introduced, this time based on the former descriptor. The main goal of the present work was to not only increase the reliability of the atom-group parameters already published in [1] but in particular to extend the number of atom groups for which as yet no parameter values have been available, with the main interest aimed at atom groups found in

ionic liquids. Besides these, parameters for a large number of additional groups with boron and silicon as central atom could be generated, thus enabling the prediction of the refractivities and polarizabilities of many boranes and silanes.

Earlier calculations of the refractivity and polarizability have been based on the bond refraction and bond polarizability, respectively, on the assumption that the molar refraction and polarizability is the sum of all the bonds in the molecule [2]. The average error between experiment and calculation was 0.7% over a number of less than 100 sample molecules. Later on, Ghose and Crippen [3] developed a method based on 110 atom types, characterized by the polarizing effect of the heteroatoms and the effect of overlapping with non-hydrogen atoms, again assuming that the sum of all the atom parameters defines the molecular descriptor value. Applying a quadratic, constrained least squares technique for the evaluation of the atom-types parameters for 504 molecules, they reported a correlation coefficient of 0.994 and a standard deviation of 1.269. Except for the parameters-calculation approach, Ghose and Crippen's method compares closely with the present one, since their atom types follow a similar principle and therefore the present results may best be compared with theirs. Another group-additivity approach was chosen by Miller [4,5] for the calculation of the molecular polarizability, whereby the atoms are defined by their state of hybridization, neglecting their neighbour atoms.

The importance of the knowledge of the refractivity and polarizability for the modelling of the dispersive and hydrophobic interactions has been outlined in detail by Ghose and Crippen [3]. The attractive forces between nonpolar compounds, also known as dispersive forces, are the result of the correlated motions of their electrons. These forces are evidently closely related to the polarizability of the molecules. Their polarizability again is linearly proportional to their refractivity, given by the Lorentz-Lorenz relation $R = 4/3\pi N\alpha$, where R is the molar refractivity, N is Avogadro's constant and α is the polarizability. Accordingly, and in contrast to our earlier calculations of the polarizability by means of the group-additivity method in [1], the present polarizabilities are directly evaluated from the molar refractivities, with the added bonus that the amount of experimental refractivity data is much larger than that of the polarity, thus enabling the prediction of molecular polarities for which in its atom-groups parameter set in [1] no atom groups are defined. It has also been shown that the molecular polarizability is directly proportional to the molecular volume [6]. Hence, on combining the polarizability/volume and polarizability/refractivity correlations, there should be a direct correlation of the refractivity with the molecular volume as postulated by Ghose and Crippen [3]. It would therefore be interesting to see if there is indeed a direct correlation of the refractivity with the "true" molecular volume as applied for the prediction of the heat capacity of solids and liquids in an earlier paper [7].

2. Method

The calculations are founded on a set of 5'988 compounds for which the experimental refractivity or polarizability data have been published, collected from a database of at present 35'952 molecules in their geometry-optimized 3D conformation, encompassing pharmaceuticals, plant protectors, dyes, ionic liquids, liquid crystals, metal-organics, intermediates, and many more, including many further experimentally determined and calculated molecular descriptors. The structural presentations have been standardized before storage by a special algorithm, ensuring that all six-membered aromatic ring systems are defined by six aromatic bonds in order to avoid structural ambiguities. In addition and for the same reason, the positive charge in amidinium, pyrazolium, and guanidinium fragments of the ionic liquids has been manually

positioned on the carbon atom between the nitrogen atoms and their C(+)-N bonds have been assumed to be aromatic, which incidentally is in better conformance with the true charge distribution in these cations, as exemplified in, e.g., Figure 1 in [8]. The analogous treatment of the carboxylate and nitro groups is not necessary, as within the present concept of atom-groups definitions they are unambiguously defined.

2.1. Definition of the Atom Groups

Details of the definition of the atom groups for use in a computer-readable form have been outlined in [1]. In Table 1 of [1], their namings and meanings have been explained; they have been retained in all the subsequent papers including the present one. However, in order to cover the successively increasing amount of additional, structurally variable molecules, several further atom groups had to be added to the parameters list. In particular, the inclusion of ordinary salts and ionic liquids as well as a number boron- and silicon-containing molecules required the corresponding atom groups listed and explained in Table 1 on some examples. These new atom groups are interpreted and processed by the computer algorithm in the same way as the remaining ones. In fact, some of these have already been applied in the calculation of the liquid viscosity of molecules in [8].

Table 1. Examples of charged or boron- or silicon-containing atom groups and their meaning

No	Atom Type	Neighbours	Meaning	Example
1	B	HN2	HBN ₂	Bis(butylamino)borane
7	B	CO2	CBO ₂	Phenyl dimethoxyborine
21	B	O3	BO ₃	Triethoxyborine
25	B(-)	C4	BC ₄ ⁻	tetracyanoborate
152	C(-) sp ³	C3	C-C ⁻ (C)-C	tricyanomethanide
245	C aromatic	H:C:N(+)	C:CH:N ⁺	C2 in pyridinium
272	C(+) aromatic	H:N2	N:C ⁺ (H):N	C2 in imidazolium
280	C sp	C#N(-)	N#C-C ⁻	tricyanomethanide
290	C sp	N#N(-)	N#C-N ⁻	dicyanoamide
295	C sp	=N=S(-)	N=C=S ⁻	Thiocyanate
316	N sp ³	HSi2	HNSi ₂	Bis(trimethoxysilyl)amine
352	N(+) sp ³	C4	NC ₄ ⁺	tetraalkylammonium
359	N(+) sp ²	O2=O(-)	NO ₃ ⁻	nitrate
363	N aromatic	C2:C(+)	C-N(C):C ⁺	N1 in 1-alkylimidazolium
365	N(+) aromatic	C:C2	C:N ⁺ (C):C	N in 1-alkylpyridinium
370	N(-)	C2	C-N ⁻ -C	dicyanoamide
398	O	CSi	COSi	Bis(trimethoxysilyl)amine
502	S4	CO=O2(-)	C-SO ₃ ⁻	Methylsulfonate
512	S4	O2=O2(-)	SO ₄ ⁻	hydrosulfate
533	Si	C3O	C ₃ SiO	Methoxytrimethylsilane
539	Si	C2N2	C ₂ SiN ₂	Diethyldiisothiocyanatosilane
554	Si	NO3	NSiO ₃	Bis(trimethoxysilyl)amine

2.2. Calculation of the Atom-Group Contributions

As outlined in [1], the parameter values of the atom groups are evaluated in four steps: in the first step those compounds for which the experimental refractivities are known are stored in a temporarily generated help list. In the second step, each molecule in the help list is broken down into its constituting "backbone" atoms (i.e. atoms bound to at least two directly bound neighbor atoms), their atom types and neighbor terms defined according to the rules detailed in [1] and then their occurrences counted. The third step involves the generation of an $M \times (N+1)$ matrix wherein M is the number of molecules, $N+1$ is the complete number of atom groups occurring plus the molecules' refractivity value, and where each matrix element (i,j) receives the number of occurrences of the jth atom group in the ith molecule. The final step comprises the normalization of this matrix into an $Ax = B$ matrix and its subsequent balancing by means of a fast Gauss-Seidel calculus [9] to receive the atom-group contributions x , which are stored and shown in Table 2, together with the corresponding statistics data at the bottom in lines A to H.

Table 2. Atom Groups and their Contribution in Refractivity Calculations

Entry	Atom Type	Neighbours	Contribution	Occurrences	Molecules
1	B	HN2	39.13	15	11
2	B	HNS	46.42	2	2
3	B	HO2	28.1	1	1
4	B	HS2	52.49	5	5
5	B	C3	66.64	4	4
6	B	C2N	62.25	8	8
7	B	C2O	64.24	22	15
8	B	C2S	69.73	10	10
9	B	CN2	58.53	2	2
10	B	CNO	59.28	1	1
11	B	CNS	65.63	1	1
12	B	CO2	61.69	31	26
13	B	COCl	48.7	4	4
14	B	CS2	72.57	8	8
15	B	CSCl	53.86	2	2
16	B	CSBr	56.93	4	4
17	B	CCl2	36.22	8	6
18	B	N3	54.93	4	2
19	B	N2O	56.24	4	2
20	B	NO2	58.3	1	1
21	B	O3	59.3	21	21
22	B	O2Cl	46.04	8	8
23	B	OCl2	33.44	6	6
24	B	S3	75.69	3	3
25	B(-)	C4	74.59	5	5
26	B(-)	O2F2	63.86	4	4
27	B(-)	F4	-2.41	18	18

28	C sp3	H3C	5.7	9421	4296
29	C sp3	H3C(+)	58.97	3	3
30	C sp3	H3N	12.24	387	246
31	C sp3	H3N(+)	19.98	76	55
32	C sp3	H3O	11.65	505	359
33	C sp3	H3S	11.49	79	55
34	C sp3	H3S(+)	16.94	2	2
35	C sp3	H3P	14.04	17	16
36	C sp3	H3P(+)	11.23	2	2
37	C sp3	H3Si	10.79	626	180
38	C sp3	H2BC	-16.41	97	53
39	C sp3	H2C2	4.63	15752	3454
40	C sp3	H2CN	11.13	1078	561
41	C sp3	H2CN(+)	18.6	223	129
42	C sp3	H2CO	10.61	2562	1560
43	C sp3	H2CS	10.63	395	253
44	C sp3	H2CS(+)	15.8	13	5
45	C sp3	H2CP	12.84	239	171
46	C sp3	H2CP(+)	12.03	46	12
47	C sp3	H2CF	5.62	33	28
48	C sp3	H2CCl	10.5	229	190
49	C sp3	H2CBr	13.44	144	127
50	C sp3	H2CJ	18.58	39	35
51	C sp3	H2CSi	9.66	345	154
52	C sp3	H2N2	17.9	2	2
53	C sp3	H2NO	18.9	1	1
54	C sp3	H2NS	17.11	1	1
55	C sp3	H2O2	16.37	19	18
56	C sp3	H2OCl	16.45	8	7
57	C sp3	H2OBr	20.6	7	7
58	C sp3	H2S2	16.43	10	5
59	C sp3	H2SCl	16.52	4	4
60	C sp3	H2SJ	21.65	2	2
61	C sp3	H2SiCl	15.47	6	5
62	C sp3	H2SiBr	18.54	4	3
63	C sp3	H2Si2	14.42	5	3
64	C sp3	HBC2	-17.46	10	7
65	C sp3	HC3	3.52	1516	1044
66	C sp3	HC2N	9.99	135	114
67	C sp3	HC2N(+)	17.27	13	13
68	C sp3	HC2O	9.55	561	462
69	C sp3	HC2P	11.84	23	21

70	C sp3	HC2S	9.55	75	53
71	C sp3	HC2F	8.42	2	2
72	C sp3	HC2Cl	9.39	84	74
73	C sp3	HC2Br	12.42	80	70
74	C sp3	HC2J	17.84	7	7
75	C sp3	HC2Si	8.64	29	15
76	C sp3	HCN2(+)	31.68	1	1
77	C sp3	HCNCl(+)	23.09	2	2
78	C sp3	HCO2	15.36	53	45
79	C sp3	HCOF	11.6	2	2
80	C sp3	HCOC1	15.53	14	9
81	C sp3	HCOBr	20.2	1	1
82	C sp3	HCS2	15.5	11	11
83	C sp3	HCSC1	14.69	1	1
84	C sp3	HCF2	5.59	29	19
85	C sp3	HCFC1	10.61	7	6
86	C sp3	HCFBr	13.45	1	1
87	C sp3	HCCl2	15.36	33	32
88	C sp3	HCClBr	18.18	5	5
89	C sp3	HCClJ	22.97	2	2
90	C sp3	HCBBr2	20.98	13	12
91	C sp3	HCBBrJ	25.95	1	1
92	C sp3	HCJ2	31.39	2	2
93	C sp3	HNO2	21.67	2	2
94	C sp3	HO3	21.51	9	9
95	C sp3	HOF2	11.17	1	1
96	C sp3	HOCl2	21.99	1	1
97	C sp3	HS3	22.99	2	2
98	C sp3	HSiCl2	20.41	5	4
99	C sp3	C4	2.47	299	251
100	C sp3	C3N	8.92	25	21
101	C sp3	C3N(+)	16.1	2	2
102	C sp3	C3O	8.42	125	113
103	C sp3	C3S	8.86	21	14
104	C sp3	C3P	11.38	1	1
105	C sp3	C3F	3.41	5	4
106	C sp3	C3Cl	8.47	7	7
107	C sp3	C3Br	11.46	7	7
108	C sp3	C3J	16.82	3	3
109	C sp3	C3Si	8.05	1	1
110	C sp3	C2NCl(+)	22.78	1	1
111	C sp3	C2O2	14.18	15	15

112	C sp3	C2OCl	14.76	4	4
113	C sp3	C2OS	14	1	1
114	C sp3	C2OP	17.43	3	3
115	C sp3	C2S2	14.73	14	14
116	C sp3	C2Si2	10.98	1	1
117	C sp3	C2F2	5.01	145	40
118	C sp3	C2FCl	9.6	3	3
119	C sp3	C2Cl2	14.26	29	26
120	C sp3	C2ClBr	17.66	3	3
121	C sp3	C2Br2	20.24	6	6
122	C sp3	C2J2	30.57	1	1
123	C sp3	CNF2	11.26	8	3
124	C sp3	CNF2(+)	19.26	2	1
125	C sp3	CO3	19.63	7	7
126	C sp3	CO2Si	17.49	1	1
127	C sp3	COF2	11.48	9	8
128	C sp3	COFCl	16.44	1	1
129	C sp3	CS3	25.53	2	2
130	C sp3	CSF2	10.98	4	3
131	C sp3	CSCl2	22.95	1	1
132	C sp3	CSiBr2	32.18	1	1
133	C sp3	CF3	5.98	98	75
134	C sp3	CF2Cl	10.67	16	14
135	C sp3	CF2Br	13.41	6	5
136	C sp3	CF2J	18.51	4	3
137	C sp3	CPF2(-)	8.9	6	2
138	C sp3	CFC12	15.39	8	6
139	C sp3	CCl3	20.42	34	31
140	C sp3	CCL2Br	23.23	3	3
141	C sp3	CBr3	29.63	4	3
142	C sp3	N2F2(+)	32.23	1	1
143	C sp3	O4	25.69	3	3
144	C sp3	OSCl2	28.62	3	3
145	C sp3	OF3	11.23	7	7
146	C sp3	OF2Cl	16.36	1	1
147	C sp3	OCl3	26.18	5	5
148	C sp3	SF3	11.78	134	72
149	C sp3	SCl3	28.7	1	1
150	C sp3	SiCl3	25.66	1	1
151	C(-) sp3	HC2	8.26	2	2
152	C(-) sp3	C3	24.54	5	5
153	C sp2	H2=C	5.49	497	428

154	C sp2	HC=C	4.53	1415	860
155	C sp2	HC=N	8.09	22	21
156	C sp2	HC=N(+)	16.04	1	1
157	C sp2	H=CN	9.75	238	132
158	C sp2	H=CN(+)	17.95	3	3
159	C sp2	H=CN(-)	-7.22	4	4
160	C sp2	HC=O	6.22	99	97
161	C sp2	H=CO	3.36	131	120
162	C sp2	H=CP	14.75	25	25
163	C sp2	H=CS	10.03	79	72
164	C sp2	H=CF	5.13	1	1
165	C sp2	H=CCl	10.29	26	23
166	C sp2	H=CBr	13.14	15	13
167	C sp2	H=CJ	18.02	2	2
168	C sp2	H=CSi	9.49	21	15
169	C sp2	HN=N	13.1	7	7
170	C sp2	HN=N(-)	5.23	2	2
171	C sp2	HN=O	11.36	11	11
172	C sp2	H=NO	6.76	3	3
173	C sp2	H=NS	13.17	2	2
174	C sp2	H=NS(+)	-1.5	11	11
175	C sp2	HN=S	20.09	1	1
176	C sp2	HO=O	5.11	25	23
177	C sp2	HO=O(-)	-0.62	4	4
178	C sp2	H=OS	12.42	2	2
179	C sp2	C2=C	3.53	377	295
180	C sp2	C2=N	6.82	41	34
181	C sp2	C2=N(+)	25.75	5	5
182	C sp2	C2=O	4.9	341	330
183	C sp2	C2=O(-)	0	4	2
184	C sp2	C2=S	11.71	1	1
185	C sp2	C=CN	8.66	44	33
186	C sp2	C=CN(+)	16.87	3	3
187	C sp2	C=CO	2.4	94	88
188	C sp2	C=CS	9.32	40	39
189	C sp2	C=CF	4.43	6	4
190	C sp2	C=CCl	9.45	51	39
191	C sp2	C=CBr	11.94	15	15
192	C sp2	C=CJ	18.24	1	1
193	C sp2	CN=N	12.41	3	3
194	C sp2	CN=N(+)	-2.61	4	4
195	C sp2	CN=O	10.15	76	71

196	C sp2	C=NO	5.46	11	11
197	C sp2	CN=O(+)	22.4	3	3
198	C sp2	=CNO(+)	18.51	1	1
199	C sp2	C=NS	12.19	3	3
200	C sp2	CO=O	3.91	1115	877
201	C sp2	CO=O(-)	-2.03	50	50
202	C sp2	C=OP	13.82	1	1
203	C sp2	C=OS	10.82	8	8
204	C sp2	C=OF	4.46	2	2
205	C sp2	C=OCl	11.16	64	55
206	C sp2	C=OBr	14.11	4	4
207	C sp2	C=OJ	20.45	1	1
208	C sp2	CS=S	19.39	1	1
209	C sp2	=CO2	1.21	2	2
210	C sp2	=COS	8	3	3
211	C sp2	=COCl	7.75	1	1
212	C sp2	=COBr	10.45	1	1
213	C sp2	=COJ	15.61	1	1
214	C sp2	=CSCl	14.74	6	4
215	C sp2	=CSBr	17.68	4	3
216	C sp2	=CSJ	22.25	1	1
217	C sp2	=CSiBr	17.13	1	1
218	C sp2	=CF2	5.09	7	7
219	C sp2	=CFCI	10.2	3	2
220	C sp2	=CCl2	15.3	15	13
221	C sp2	=CClJ	22.87	1	1
222	C sp2	=CBr2	20.76	7	7
223	C sp2	=CBrJ	25.82	1	1
224	C sp2	=CJ2	30.75	1	1
225	C sp2	N2=N	16.88	2	2
226	C sp2	N2=O	14.77	10	10
227	C sp2	N2=S	21.5	2	2
228	C sp2	NO=O	9.3	19	16
229	C sp2	NO=S	18.4	1	1
230	C sp2	N=OS	17.32	2	2
231	C sp2	N=OCl	16.29	1	1
232	C sp2	=NOCl	10.4	1	1
233	C sp2	=NS2	20.87	3	3
234	C sp2	=NSCl	17.86	1	1
235	C sp2	=NSBr	21.65	1	1
236	C sp2	O2=O	2.9	21	20
237	C sp2	O=OS	-14.19	1	1

238	C sp ²	O=OCl	10	13	12
239	C sp ²	=OS ₂	17.71	1	1
240	C sp ²	OS=S	18.21	8	8
241	C sp ²	S ₂ =S	26.78	2	2
242	C sp ²	=OSCl	17.33	1	1
243	C aromatic	H:C ₂	4.42	6519	1357
244	C aromatic	H:C:N	6.45	139	92
245	C aromatic	H:C:N(+)	3.24	62	33
246	C aromatic	H:N ₂	7.84	3	3
247	C aromatic	B:C ₂	-16.99	46	37
248	C aromatic	:C ₃	4.56	251	119
249	C aromatic	C:C ₂	3.53	1300	909
250	C aromatic	C:C:N	5.73	52	43
251	C aromatic	C:C:N(+)	2.09	6	5
252	C aromatic	:C ₂ N	9.79	158	143
253	C aromatic	:C ₂ N(+)	18.25	40	35
254	C aromatic	:C ₂ :N	6.2	11	11
255	C aromatic	:C ₂ O	2.8	359	287
256	C aromatic	:C ₂ P	11.21	35	34
257	C aromatic	:C ₂ S	9.77	43	40
258	C aromatic	:C ₂ F	4.32	119	64
259	C aromatic	:C ₂ Cl	9.24	123	99
260	C aromatic	:C ₂ Br	12.01	60	54
261	C aromatic	:C ₂ J	16.99	19	18
262	C aromatic	:C ₂ Si	8.57	79	52
263	C aromatic	:CN:N	11.15	3	2
264	C aromatic	C:N ₂	8.01	4	2
265	C aromatic	:C:NO	5.39	4	4
266	C aromatic	:C:NF	6.07	5	4
267	C aromatic	:C:NCl	11.5	3	3
268	C aromatic	:C:NBr	13.99	2	2
269	C aromatic	:C:NJ	20.37	1	1
270	C aromatic	N:N ₂	15.39	5	2
271	C aromatic	:N ₂ Cl	12.28	1	1
272	C(+) aromatic	H:N ₂	-10.11	95	95
273	C(+) aromatic	C:N ₂	-64.74	3	3
274	C(+) aromatic	:N ₃	-8.28	5	5
275	C sp	B#N(-)	-14.24	20	5
276	C sp	H#C	4.41	84	77
277	C sp	=C ₂	4.9	9	9
278	C sp	C#C	3.88	200	138
279	C sp	C#N	5.49	149	132

280	C sp	C#N(-)	-3.13	15	5
281	C sp	=C=O	5.84	4	3
282	C sp	#CO	3.2	6	6
283	C sp	#CS	9.65	1	1
284	C sp	#CSi	8.08	6	3
285	C sp	#CCl	10.37	3	3
286	C sp	#CBr	12.31	4	4
287	C sp	#CJ	17.16	6	6
288	C sp	=N2	11.03	1	1
289	C sp	N#N	10.62	3	3
290	C sp	N#N(-)	1.34	26	13
291	C sp	=N=O	8.24	18	14
292	C sp	#NO	5.66	1	1
293	C sp	#NP	-2.29	1	1
294	C sp	=N=S	15.8	34	20
295	C sp	=N=S(-)	7.85	4	4
296	C sp	#NS	11.5	12	12
297	N sp3	H2B	-12.94	1	1
298	N sp3	H2C	-2	148	133
299	N sp3	H2C(pi)	-1.3	77	69
300	N sp3	H2N	-5.01	13	13
301	N sp3	H2Si	1.97	4	4
302	N sp3	HC2	-9.63	110	108
303	N sp3	HBC	-20.05	18	11
304	N sp3	HBC(pi)	-18.67	6	5
305	N sp3	HC2(pi)	-8.63	54	53
306	N sp3	HC2(2pi)	-7.37	37	34
307	N sp3	HCN	-2.94	9	5
308	N sp3	HCN(pi)	-1.31	2	2
309	N sp3	HCN(+)(pi)	4.48	2	2
310	N sp3	HCN(2pi)	-3.61	3	3
311	N sp3	HCO	-2.67	2	2
312	N sp3	HCP	0.72	3	3
313	N sp3	HCSi	-5.5	6	6
314	N sp3	HCSi(pi)	-4.28	1	1
315	N sp3	HNSi	-8.36	34	19
316	N sp3	HSi2	-1.34	19	15
317	N sp3	B2C	-38.6	12	4
318	N sp3	BC2	-27.51	16	11
319	N sp3	BC2(pi)	-26.43	2	1
320	N sp3	C3	-16.75	123	110
321	N sp3	C3(pi)	-15.83	67	61

322	N sp3	C3(2pi)	-14.97	22	22
323	N sp3	C3(3pi)	-15.13	3	3
324	N sp3	C2N	-0.73	45	30
325	N sp3	C2N(pi)	-0.19	14	14
326	N sp3	C2N(2pi)	-10.64	4	4
327	N sp3	C2N(3pi)	-9.23	2	2
328	N sp3	C2N(+)(pi)	-2.99	2	2
329	N sp3	C2N(+)(2pi)	-1.57	2	2
330	N sp3	C2N(+)(3pi)	-40.57	5	5
331	N sp3	C2O	-10.11	4	4
332	N sp3	C2P	-6.55	86	54
333	N sp3	C2Si	-12.89	27	12
334	N sp3	CCl2(pi)	11.05	1	1
335	N sp2	H=C	1.03	8	8
336	N sp2	C=C	-6.59	63	58
337	N sp2	C=N	-2.23	11	6
338	N sp2	C=N(+)	0.41	5	5
339	N sp2	=CN	-0.2	19	13
340	N sp2	=CN(-)	13.22	2	2
341	N sp2	=CO	-2.21	34	33
342	N sp2	=CP	2.65	1	1
343	N sp2	=CS	4.72	3	2
344	N sp2	=CSi	-2.01	26	12
345	N sp2	N=N	3.04	1	1
346	N sp2	N=O	-4.93	12	12
347	N sp2	O=O	3.41	18	15
348	N sp2	P=P	4.02	9	3
349	N(+) sp3	H3C	-0.39	13	13
350	N(+) sp3	H2C2	-15.27	4	4
351	N(+) sp3	HC3	-30.15	8	8
352	N(+) sp3	C4	-47.94	46	46
353	N(+) sp2	HC=C	12.52	4	4
354	N(+) sp2	C2=C	-5.91	11	11
355	N(+) sp2	C=CN	0	5	5
356	N(+) sp2	C=NO(-)	-4.48	2	2
357	N(+) sp2	CO=O(-)	-7.16	75	65
358	N(+) sp2	NO=O(-)	0	6	6
359	N(+) sp2	O2=O(-)	0.2	27	20
360	N aromatic	H2:C(+)	0	5	5
361	N aromatic	HC:C(+)	10.05	1	1
362	N aromatic	:C2	-1.94	120	105
363	N aromatic	C2:C(+)	1.26	205	103

364	N aromatic	:C:N	0.2	6	3
365	N(+) aromatic	C:C2	-1.86	33	33
366	N(+) aromatic	:C2O(-)	8.85	1	1
367	N(+) sp	C#C(-)	-7.99	3	3
368	N(+) sp	=C=N(-)	-3.91	1	1
369	N(+) sp	=N2(-)	2.99	3	3
370	N(-)	C2	4.69	15	15
371	N(-)	CN	-12.52	2	2
372	N(-)	S2	1.69	69	69
373	O	HB	-17.09	3	3
374	O	B2	-35.49	6	6
375	O	HC	-3.5	602	527
376	O	HC(pi)	3.39	266	250
377	O	HN	2.35	4	4
378	O	HN(pi)	4.33	14	14
379	O	HO	2.75	15	15
380	O	HS	7.17	5	4
381	O	HP	5.14	26	23
382	O	HSi	0.8	7	7
383	O	BC	-23.16	165	75
384	O	BC(pi)	-11.65	2	1
385	O	BC(-)(pi)	-31.4	8	4
386	O	C2	-10.27	617	420
387	O	C2(pi)	-3.51	1209	958
388	O	C2(2pi)	3.23	137	135
389	O	CN	-4.7	2	2
390	O	CN(pi)	-2.22	31	28
391	O	CN(+)(pi)	2.51	24	17
392	O	CN(2pi)	3.03	5	5
393	O	CO	-3.92	31	23
394	O	CO(pi)	3.65	2	2
395	O	CP	-1.46	471	249
396	O	CP(pi)	4.87	50	30
397	O	CS	-0.98	48	37
398	O	CSi	-6.31	244	103
399	O	CSi(pi)	0.28	29	19
400	O	CCl	2.14	1	1
401	O	N2(2pi)	3.14	1	1
402	O	P2	7.2	23	19
403	O	Si2	-2.39	116	35
404	P3	H2C	2.85	17	17
405	P3	HC2	-6.24	3	3

406	P3	C3	-15.17	18	18
407	P3	C2O	-10.92	10	10
408	P3	C2S	-3.08	3	3
409	P3	C2Cl	-6.82	16	16
410	P3	CO2	-6.82	15	15
411	P3	COCl	-2.2	6	6
412	P3	CS2	17.67	1	1
413	P3	CCl2	12.05	8	8
414	P3	N3	-4.26	1	1
415	P3	N2O	-2.29	3	3
416	P3	NO2	-1.46	3	3
417	P3	O3	-1.41	26	26
418	P3	O2Cl	6.11	1	1
419	P3	OCl2	16.38	1	1
420	P3	S3	21.45	4	4
421	P4	HC2=O	-7.52	2	2
422	P4	HO2=O	2.18	17	17
423	P4	HO2=S	8.79	3	3
424	P4	C3=O	-17.18	3	3
425	P4	C3=S	-8.85	3	3
426	P4	C2O=O	-12.11	10	10
427	P4	C2O=O(-)	-15.97	1	1
428	P4	C2=OS	-4.17	1	1
429	P4	C2O=S	-4.41	1	1
430	P4	C2S=S	-0.38	1	1
431	P4	C2=SCl	5.18	1	1
432	P4	CN2=O	-10.68	10	10
433	P4	CNO=O	8.01	1	1
434	P4	CN=OF	-5.4	4	4
435	P4	CN=OCl	0.56	5	5
436	P4	CO2=O	-7.79	42	42
437	P4	CO2=O(-)	-10.36	1	1
438	P4	CO2=S	0.26	8	8
439	P4	C=OS2	8.61	2	2
440	P4	COS=S	7.49	30	30
441	P4	C=OF2	0.52	5	5
442	P4	C=OCl2	11.1	9	9
443	P4	CS2=S	16.66	6	3
444	P4	C=SCl2	19.41	5	5
445	P4	N3=O	-6.3	1	1
446	P4	N2O=O	-5	5	5
447	P4	N=NO2	-3.25	6	2

448	P4	N2O=S	3.2	2	2
449	P4	N2=OF	-0.37	1	1
450	P4	N=NS2	12.33	3	1
451	P4	NO2=O	-4.03	3	3
452	P4	NO2=S	4.11	6	6
453	P4	NO=OF	0.12	7	6
454	P4	NO=SF	7.56	5	4
455	P4	N=OF2	4.05	1	1
456	P4	N=OFCl	9.6	2	2
457	P4	N=OFBr	12.55	1	1
458	P4	N=OCl2	14.9	1	1
459	P4	N=SFCl	17.24	1	1
460	P4	N=SFBr	20.83	1	1
461	P4	N=SCl2	22.78	1	1
462	P4	O3=O	-2.5	33	26
463	P4	O3=O(-)	-6.33	3	3
464	P4	O3=S	5.03	16	14
465	P4	O2=OS	15.08	4	4
466	P4	O2=OF	1.56	16	12
467	P4	O2=OCl	6.38	2	2
468	P4	O2S=S	12.87	2	2
469	P4	O2=SF	9.65	2	1
470	P4	O2=SCl	14.28	3	3
471	P4	O=OF2	5.45	1	1
472	P4	O=OFCl	10.51	7	6
473	P4	O=OFBr	13.17	1	1
474	P4	O=OCl2	15.86	1	1
475	P4	O=SF2	12.58	1	1
476	P4	O=SFCl	18.16	1	1
477	P4	O=SFBr	21.4	1	1
478	P4	O=SCl2	23.03	1	1
479	P(-)	C3F3	-11.9	2	2
480	P(-)	F6	1.32	6	6
481	P(+)	C4	-14.3	12	12
482	S2	HC	2.74	78	58
483	S2	HC(pi)	2.64	8	7
484	S2	HP	5.84	27	27
485	S2	BC	-21.7	51	32
486	S2	BC(pi)	-21.88	3	3
487	S2	C2	-4.08	157	98
488	S2	C2(pi)	-3.93	77	73
489	S2	C2(2pi)	-4.31	70	70

490	S2	CP	-1.63	34	18
491	S2	CS	2.06	38	21
492	S2	CS(pi)	-12.06	2	1
493	S2	CCl	6.16	5	5
494	S2	N2(2pi)	-5.14	1	1
495	S2	PCl	0	4	4
496	S2	P2	0	6	3
497	S2	S2	8.87	6	5
498	S4	C2=O	-3.2	4	4
499	S4	C2=O2	-3.24	12	12
500	S4	CN=O2(-)	-0.22	126	63
501	S4	CO=O2	-1.48	11	11
502	S4	CO=O2(-)	-3.78	24	24
503	S4	C=OCl	9.42	6	6
504	S4	C=OS	3.69	4	4
505	S4	C=O2F	4.69	8	8
506	S4	C=O2Cl	8.91	8	8
507	S4	N=O2F(-)	5.76	12	6
508	S4	N=O2Cl	10.28	1	1
509	S4	O=OCl	11.86	1	1
510	S4	O2=O	1.31	7	7
511	S4	O2=O2	1.17	4	4
512	S4	O2=O2(-)	-2.26	16	16
513	S4	O=O2Cl	11.45	2	2
514	S4	O=O2F	5.93	1	1
515	S(+)	C3	-19.18	5	5
516	Si	H3C	6.42	8	7
517	Si	H3Si	12.32	19	8
518	Si	H2C2	0.06	12	10
519	Si	H2CN	6.65	1	1
520	Si	H2CCl	10.82	1	1
521	Si	H2Si2	12.04	18	7
522	Si	HC3	-6.7	14	14
523	Si	HC2N	0.57	5	4
524	Si	HC2O	-0.27	11	7
525	Si	HC2Cl	3.98	4	4
526	Si	HCN2	7.39	6	6
527	Si	HCO2	5.89	18	9
528	Si	HCOCl	10.13	1	1
529	Si	HN3	14.51	1	1
530	Si	HSi3	12.05	3	3
531	Si	C4	-12.83	49	40

532	Si	C3N	-6.05	42	32
533	Si	C3O	-6.7	84	61
534	Si	C3F	-7.57	5	5
535	Si	C3Cl	-2.55	12	12
536	Si	C3Br	0.52	3	3
537	Si	C3J	6.46	2	2
538	Si	C3Si	-6.69	6	3
539	Si	C2N2	1.02	12	10
540	Si	C2O2	-0.54	100	39
541	Si	C2Si2	-0.39	3	2
542	Si	C2SiCl	3.56	2	1
543	Si	C2F2	-2.89	6	6
544	Si	C2Cl2	8.03	13	13
545	Si	C2Br2	14.34	1	1
546	Si	C2J2	26	1	1
547	Si	CN3	7.74	6	6
548	Si	CN2Cl	11.22	2	2
549	Si	CO3	5.81	30	30
550	Si	COCl2	14.59	4	4
551	Si	CF3	2.56	3	3
552	Si	CCl3	18.65	17	16
553	Si	CBr3	27.76	1	1
554	Si	NO3	12.84	6	4
555	Si	N2O2	4.42	1	1
556	Si	N3O	0.43	1	1
557	Si	N4	14.64	4	4
558	Si	O4	12.5	15	15
559	Si	O3Cl	16.78	1	1
560	Si	OCl3	25.14	2	2
561	Chloride		-1	7	7
562	Bromide		3.11	3	3
A	Based on	Valid groups	382		5988
B	Goodness of fit	R ²	0.9997		5763
C	Deviation	Average	0.29		5763
D	Deviation	Standard	0.38		5763
E	K-fold cv	K	10		5572
F	Goodness of fit	Q ²	0.9997		5572
G	Deviation	Average (cv)	0.31		5572
H	Deviation	Standard (cv)	0.41		5572

2.3. Calculation of the Refractivity

The calculation of the refractivity of a molecule, based on the atom-group parameters compiled in Table 2, is a simple summing up of the contribution of each atom group found in a molecule, as exemplified in Table 3 for 1-butyl-3-methylimidazolium tetrafluoroborate (Fig. 1), for which the experimentally evaluated refractivity value was 47.81 [10]. The parameters for the monoatomic anions found among some ILs are given under the respective "group" names "Chloride" and "Bromide". Any further halogenide anion can be taken into account analogously as soon as the experimental data of at least three representative compounds are available.

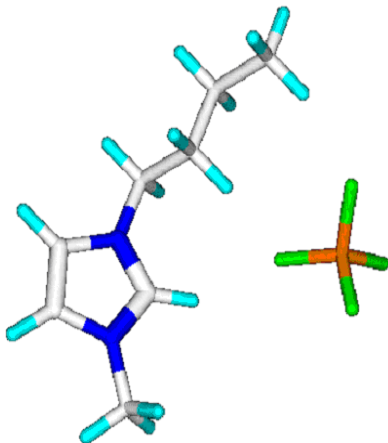


Fig. 1. 1-Butyl-3-methylimidazolium tetrafluoroborate

Table 3. Example calculation of the refractivity of 1-butyl-3-methylimidazolium tetrafluoroborate

Atom type	B(-)	C sp3	C sp3	C sp3	C sp3	C sp2	C(+) aromatic	N aromatic	Sum
Neighbors	F4	H3C	H3N	H2C2	H2CN	H=CN	HN2	C2:C(+)	
Contribution	-2.41	5.7	12.24	4.63	11.13	9.75	-10.11	1.26	
n Groups	1	1	1	2	1	2	1	2	
n x Contribution	-2.41	5.7	12.24	9.26	11.13	19.5	-10.11	2.52	47.83

It goes without saying that this calculation method is limited to compounds for which each atom group is defined by a parameter value in Table 2. In addition, as the reliability of these parameter values increases with the number of independent molecules upon which they are based, only atom groups should be considered for which the number of molecules in the rightmost column of Table 2 is three or more, which are henceforth called "valid". (It could be shown by means of several cross-validation calculations that the decrease of the cross-validated standard deviation on going from three to four molecules per atom group is insignificant compared with the decrease observed when going from two to three molecules per atom group.) Consequently, the number of molecules for which the refractivity values have been calculated (lines B, C and D in Table 2) is necessarily smaller than the number upon which the calculation of the complete set of parameters is based (line A in Table 2).

2.4. Cross-Validation Calculations

The calculations of the atom-group parameters are immediately followed by a plausibility test applying a 10-fold cross-validation algorithm comprising 10 recalculations omitting in each case a different tenth of the complete set of compounds, ensuring that each compound has been used once as a test sample. The resulting training and test data are added to the molecule's datafiles. Finally, the corresponding statistics data are evaluated and collected at the bottom of Table 2. Due to the smaller number of training molecules in the cross-validation calculations and the condition that only atom-group parameters should be considered in the calculation of the individual refractivities for which the number of molecules in the rightmost column is three or more, the number of molecules with calculated refractivities (lines E, F, G and H) is again lower in the test set than in the training set (lines B, C and D). Atom-group parameters with molecule numbers below three in the rightmost column, which are accordingly at present not applicable for refractivity calculations, have deliberately been left in Table 2 for future use in this continuing project and not least in the hope that interested scientists may assist in increasing the number of “valid” groups in this parameters list by compounds carrying the underrepresented atom groups. At present, the list of elements for refractivity/polarizability calculations is limited to H, B, C, N, O, P, S, Si, and/or halogen, but is easily extendable to enable the parametrization of atom groups containing additional elements for which experimental densities and refractive indices are available.

2.5. Calculation of the Polarizability

According to the Lorentz-Lorenz relation $R = 4/3\pi N\alpha$, N being Avogadro's number, the refractivity R of a molecule can be translated into its polarizability α by simply multiplying its refractivity value with the reciprocal value of $4/3\pi N$, which is 0.3964, if the refractivity is expressed in mL and the polarizability in $\text{\AA}^3$. Therefore in this study, for each input experimental refractivity value, the corresponding polarizability value has also been evaluated and stored as experimental value in the database, and vice versa. The latter is all the more justified as in many (if not most) cases the polarizability value has been evaluated via the refractivity value. Accordingly, the number of experimental data for these two descriptors is identical, and so is their list of atom-group parameters. As a consequence, calculation of a molecule's refractivity value by means of the group-additivity method, based on the refractivity parameters in Table 2, immediately enabled the calculation of its polarizability value by simply multiplying it with 0.3964.

3. Sources of Refractivity and Polarizability Data

In most cases, it was not the refractivity value itself that was published in the following references but the refractive index (n_d) and the density (d) of the molecules, which then had to be translated into the refractivity (R) according to the equation $R = (n_d^2 - 1)/(n_d^2 + 2) \times (M/d)$, where M is the molecular weight. The primary sources of the refractivity data for the earlier [1] as well as the present study were the comprehensive CRC Handbook of Chemistry and Physics [11] and the collective work of Ghose and Crippen [12]. Within the last 7 years since the first publication dealing with the present subject however, a large number of further papers has been collected producing additional refractivity and polarizability data which helped to extend the scope of applicability of the atom-group additivity method, particularly for boron- and silicon-containing compounds and ionic liquids. In the following, they have been sorted by their dominant functional features. Within the last ca. 85 years, many papers have been published producing the refractive indices and densities to characterize various hydrocarbons [13-34], alcohols [35-42], ethers [43-47], acids [48],

(ortho)esters and carbonates [49-62], acetals [63,64], ketones [65,66], peroxides [67-71], amines, hydrazines, nitriles and nitro compounds [72-78], various boron- [79-97], phosphorus- [98-137] and sulfur-containing compounds [138-162]. Many of the compounds mentioned so far also carried halogens [163-199]. An interesting extension to the parameters database was provided by papers presenting results of silicon-containing compounds [200-243]. Beyond the refractivity data of the various mentioned functional groups those for a number of hetarenes and heterocycles have been published [244-263]. Another important extension that has not been covered in the earlier paper [1] is the class of ionic liquids [10,264-370]. In addition, several papers have been added which contributed various subjects that could not be assigned to any specific subject of the aforementioned ones [2,371-389]. Finally, a number of papers published experimental data of the polarizability of molecules, in many cases derived from their refractivity values [6,390-401].

4. Results

4.1. Refractivity

In the paper of Ghose and Crippen [3] mentioned earlier, it was stated that the molar refractivity is directly related to the molecule's volume, expressed in the refractivity's unit "mL", their atom-group parameters accordingly being associated with the volume of the molecule's constituting atoms. The present approach, on the other hand, does not care about the theoretical background of the refractivity as it is a purely mathematical method to adjust the calculated to the experimental data, and therefore the resulting atom-group parameters must not be assigned with any physical meaning. Consequently, as can be seen in Table 2 and 3, negative parameter values are not unusual.

While in the earlier paper [1] generally no limit was given concerning the deviation of the experimental data from the calculated ones for the evaluation of the group-atom parameters, in the present work the atom-group parameters in Table 2 and the statistics data at its bottom (Lines A to H) are the result after a stepwise elimination of outliers, defined as their experimental value deviating from the calculated one by more than three times the cross-validated standard error Q^2 . The final list of discarded outliers is available in the Supplementary Materials. As a consequence, 5'988 of the originally 6'501 compounds with experimental data remained for the evaluation of said parameters, leaving ca. 7.9% as outliers. Due to the elimination of the outliers the statistical data have significantly improved in comparison with those in the earlier paper: not only is the present set of parameters based on a significantly larger number of molecules (5'988 vs. 4'300, rows A in Tables 2 and 13 of [1]) and a larger number of atom groups (562 vs. 364), but also their standard deviation (0.38 vs. 0.66, rows D) and the cross-validated deviation (0.41 vs. 0.7, rows H) have drastically improved. Together with the corresponding correlation coefficients R^2 and Q^2 of 0.9997 (rows B and F in Table 2) in the present work, they compare very favourably with the correlation coefficient of 0.994 and the standard deviation of 1.269 published by Ghose and Crippen [3]. The mean absolute percentage deviation (MAPD) of the finally calculated refractivities from the experimental values of 5'988 molecules is 0.76%. The increased number of "valid" atom-group parameters enabled the calculation of the refractivities and polarizabilities of ca. 80% of the close to 36'000 molecules in the present database, which can be viewed as representative for the entire chemical realm. The excellent correlation between experiment and prediction is visualized in the correlation diagram of Fig. 2. The corresponding histogram in Fig. 3 confirms the uniform distribution of the deviations between the experimental and calculated refractivities, their experimental values ranging from 8.23 (methanol) to 271.13 (glycerol tristearate). The complete set of compounds with experimental refractivities

used for the group-atom parameters of Table 2 are available in the Supplementary Materials.

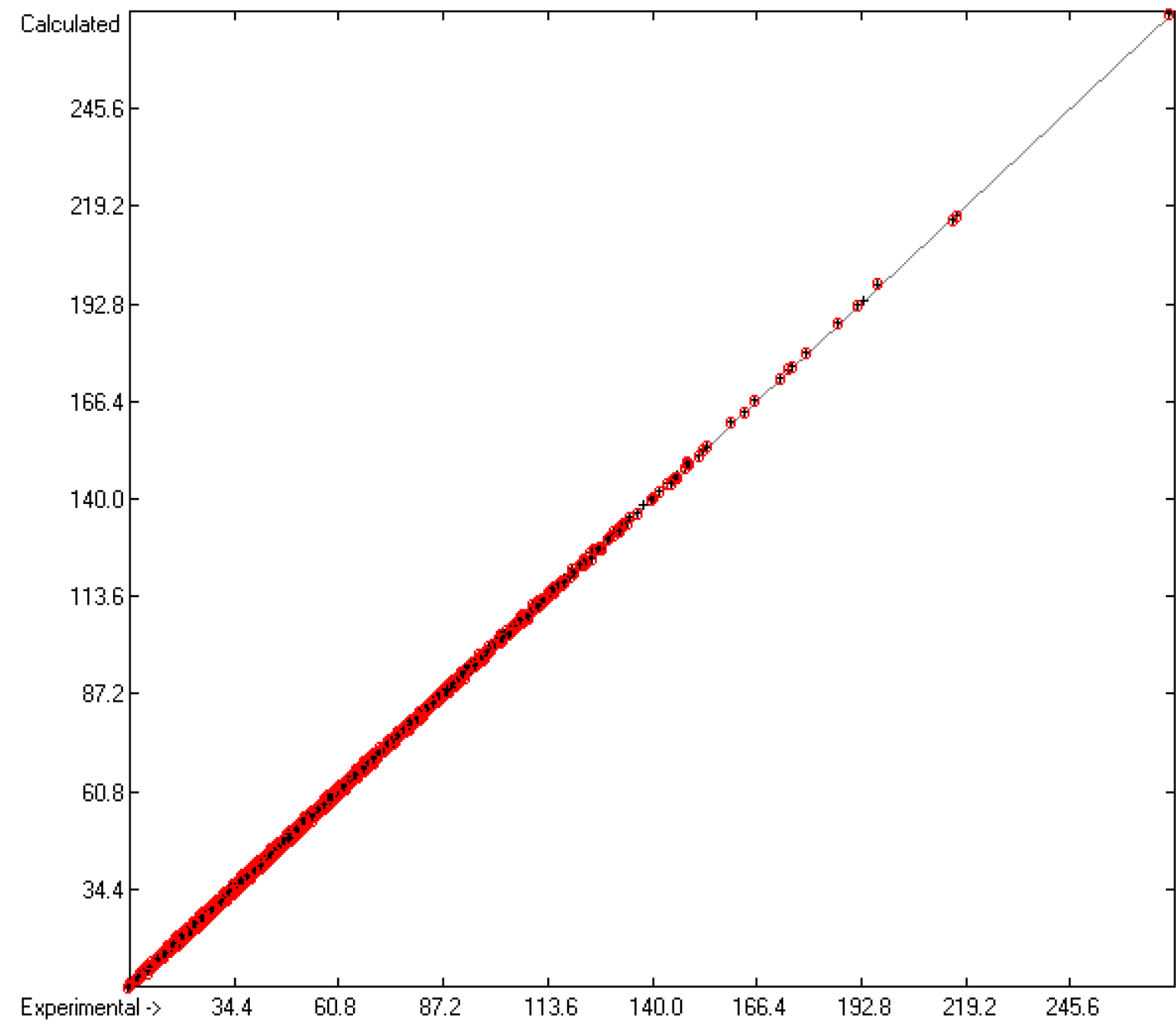


Figure 2. Correlation diagram of the refractivity data. Cross-validation data are superpositioned as red circles. (10-fold cross-valid.: N=5763, $Q^2=0.9997$, regression line: intercept=0.0292; slope=0.9995, MAPD=0.76%).

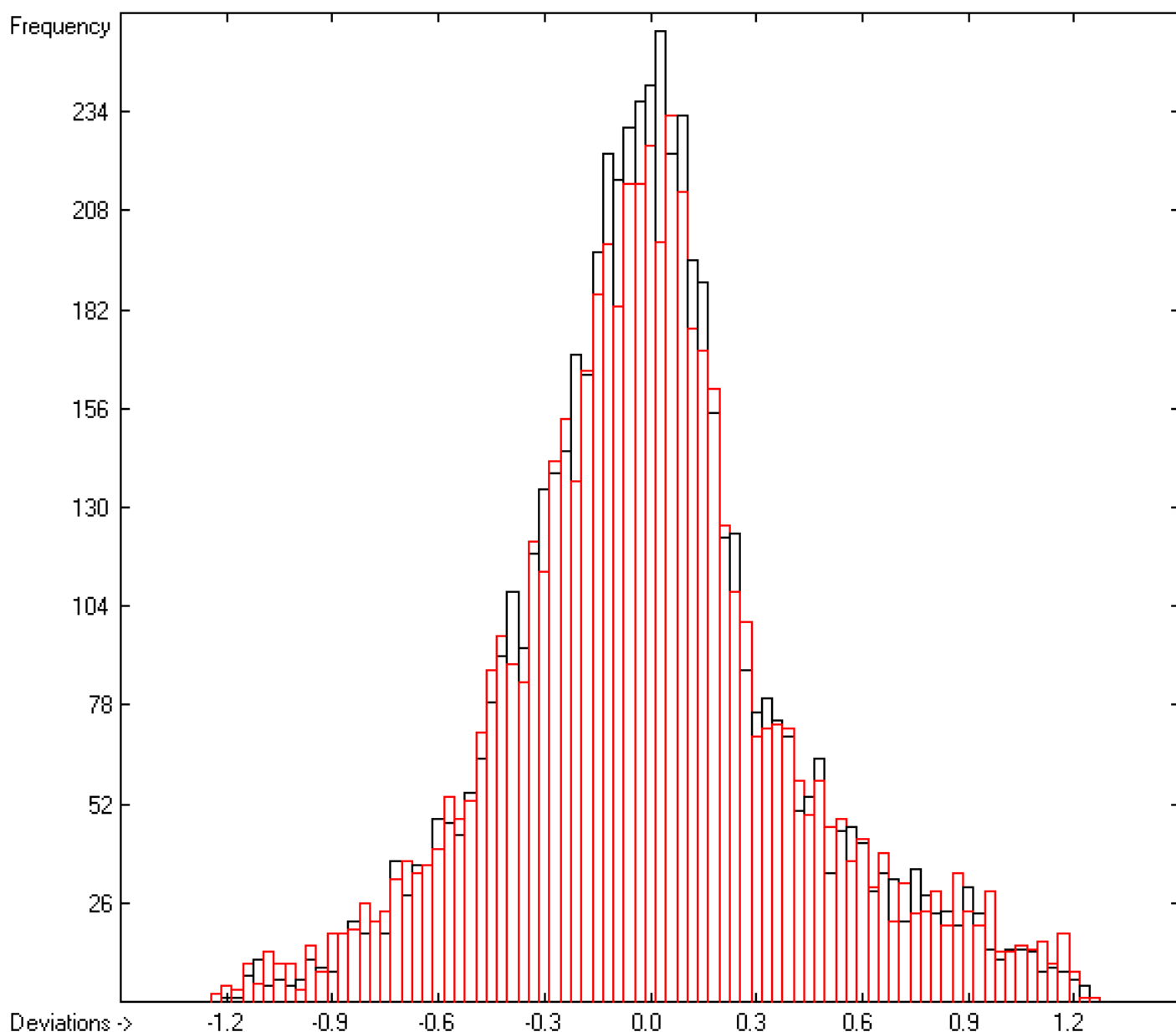


Figure 3. Histogram of the refractivity data. Cross-validation data are superpositioned as red bars. ($\sigma = 0.38$; $S = 0.41$; experimental values range from 8.23 to 271.13).

An interesting observation can be made with respect to the outliers in that many of them are solids. Cao et al. [402] have shown that solid compounds can exhibit up to three differing refractive indices, depending on their crystal symmetry. A typical example is Ibuprofen, a non-steroidal antirheumatic, which shows the three refractive index values 1.522, 1.572 and 1.644. With its reported density of 1.119 g/cm^3 and a refractivity of 60.95, calculated by means of our group-additivity model, we calculated a refractive index of 1.575, which is pretty close to the mean of the three experimental values. Analogous results have been found with several other outliers, confirming the assessment that in cases where the experimental refractive index strongly deviates from the predicted one, the reason might be that a specific crystal form of the compound has been examined. Since these mean refractive index values usually do not represent real crystalline forms, they have not been included in the group-parameters optimization procedure.

Since the last paper [1] of 2015, the systematic screening of the chemical literature has provided a number of refractivities data of previously under-represented classes of molecules enabling, as mentioned

earlier, a substantial increase of the number of atom-group parameters in the present Table 2 compared with the one of Table 13 in [1]. In particular, three classes of compounds have experienced an extended representation and will in the following be discussed in more detail: ionic liquids, and silicon- and boron-containing compounds.

4.1.1. Ionic Liquids

In the last ca. 25 years, ionic liquids (ILs) have experienced increasing attention as potential replacements for volatile solvents as they are non-volatile, non-inflammable and can easily be recycled. Their physical properties are easily tunable by suitable choice of their cation and anion, making them favorable candidates as media for chemical syntheses. The enormous variety of potential cation-anion combinations, however, obliges one to put the focus on those candidates with the most promising properties. In the last few years a substantial number of ILs have been synthesized and their physical properties have been examined. Based on these results, few attempts have been made so far to utilize these results for the prediction of the physical properties of as yet unknown cation-anion combinations, and if yes, then for a narrow scope within the scientists' range of experience (see e. g. Almeida et al. [320]), or as in other cases, as e. g. in the papers of Sattari et al. [338] or of Venkatraman et al. [363], for the prediction of a specific property based on a fairly large range of ILs by either applying quantitative structure-property relationship (QSPR) technique or machine learning. The present atom-group additivity approach, on the other hand, has proven its versatility in that it is able to predict a number of properties of nearly any type of compound by means of an identical algorithm, simply using the appropriate atom-group parameters tables. Accordingly, based on the updated parameters tables in this ongoing project, we have been able to calculate the heat of combustion [403] for 30 ILs with a correlation coefficient R^2 of 1.0 and a mean average percentage deviation from experimental values (MAPD) of 0.21%, the heat of vaporization [404] of 61 ILs ($R^2=0.9615$, MAPD=2.12%), the liquid viscosity [8] for 93 ILs ($R^2=0.9823$, MAPD=3.24%), the surface tension [405] of 160 ILs ($R^2=0.8478$, MAPD=5.1%), and the liquid heat capacity at 293K [406] of 140 ILs ($R^2=0.9986$, MAPD=1.05%). In analogy to these results, the refractivity values of 228 ILs calculated by means of the atom-group parameters of Table 2 have been compared with their experimental data and collected alphabetically in Table 4, revealing a MAPD of only 0.44%.

Table 4. Calculated and experimental refractivity of ionic liquids

Molecule name	Refractivity exp	Refractivity calc	Deviation	Dev. in %
1-(2-Cyanoethyl)-3-(2-hydroxyethyl)-imidazolium chloride	51.06	50.40	0.66	1.29
1-(2-Cyanoethyl)-3-(2-propen-1-yl)-imidazolium chloride	53.46	53.31	0.15	0.28
1-(2-Cyanoethyl)-3-octylimidazolium 3-sulfobenzoate	111.59	112.27	-0.68	-0.61
1-(2-Hydroxyethyl)-3-methylimidazolium perfluoropentanoate	62.30	61.37	0.93	1.49
1-(3-Cyanopropyl)-3-methylimidazolium bis(trifluoromethylsulfonyl) amide	74.64	74.84	-0.20	-0.27

1-(3-Cyanopropyl)-3-methylimidazolium dicyanamide	56.96	57.40	-0.44	-0.77
1-(3-Cyanopropyl)-3-methylimidazolium tetrafluoroborate	46.88	47.62	-0.74	-1.58
1-(3-Cyanopropyl)-pyridinium bis(trifluoromethylsulfonyl) amide	75.74	76.04	-0.30	-0.40
1-(3-Cyanopropyl)-pyridinium dicyanamide	57.75	58.60	-0.85	-1.47
1,1,3,3-Tetramethylguanidinium butanoate	56.23	56.13	0.10	0.18
1,1,3,3-Tetramethylguanidinium heptanoate	70.63	70.02	0.61	0.86
1,1,3,3-Tetramethylguanidinium hexanoate	64.74	65.39	-0.65	-1.00
1,1,3,3-Tetramethylguanidinium octanoate	74.36	74.65	-0.29	-0.39
1,1,3,3-Tetramethylguanidinium pentanoate	60.85	60.76	0.09	0.15
1,2-Diethylpyridinium ethylsulfate	64.48	64.43	0.05	0.08
1,3-Diethylimidazolium bis(trifluoromethylsulfonyl) amide	70.29	70.38	-0.09	-0.13
1,3-Dimethylimidazolium bis(trifluoromethylsulfonyl) amide	60.56	61.20	-0.64	-1.06
1,3-Dimethylimidazolium methosulfate	44.78	44.80	-0.02	-0.04
1,3-Dipropylimidazolium bis(trifluoromethylsulfonyl) amide	79.71	79.64	0.07	0.09
1-Benzyl-3-methylimidazolium bis(trifluoromethylsulfonyl) amide	85.86	85.72	0.14	0.16
1-Butyl-1-methylpiperidinium bis(trifluoromethylsulfonyl)amide	81.48	81.50	-0.02	-0.02
1-Butyl-1-methylpyrrolidinium 2-acryloamido-2-methylpropanesulfonate	91.47	90.77	0.70	0.77
1-Butyl-1-methylpyrrolidinium acetate	55.00	55.73	-0.73	-1.33
1-Butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide	76.89	76.87	0.02	0.03
1-Butyl-1-methylpyrrolidinium dicyanamide	60.12	59.43	0.69	1.15
1-Butyl-1-methylpyrrolidinium methylsulfate	60.93	60.47	0.46	0.75
1-Butyl-1-methylpyrrolidinium trifluoromethanesulfonate	60.44	60.06	0.38	0.63
1-Butyl-2,3-dimethylimidazolium bis(trifluoromethanesulfonyl) amide	79.33	79.39	-0.06	-0.08
1-Butyl-2,3-dimethylimidazolium tetrafluoroborate	52.38	52.17	0.21	0.40
1-Butyl-2-methylpyridinium tetrafluoroborate	53.45	53.58	-0.13	-0.24
1-Butyl-3-(2-cyanoethyl)-imidazolium chloride	57.93	58.25	-0.32	-0.55
1-Butyl-3-(2-cyanoethyl)imidazolium thiocyanate	67.06	67.10	-0.04	-0.06
1-Butyl-3-ethylimidazolium bis(trifluoromethylsulfonyl) amide	79.44	79.64	-0.20	-0.25
1-Butyl-3-ethylimidazolium triflate	63.01	62.83	0.18	0.29

1-Butyl-3-methylimidazolium 2-acryloamido-2-methylpropanesulfonate	88.52	88.95	-0.43	-0.49
1-Butyl-3-methylimidazolium acetate	54.18	53.91	0.27	0.50
1-Butyl-3-methylimidazolium bis(perfluorobutanesulfonyl) amide	105.39	105.45	-0.06	-0.06
1-Butyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	74.99	75.05	-0.06	-0.08
1-Butyl-3-methylimidazolium dicyanoamide	57.80	57.61	0.19	0.33
1-Butyl-3-methylimidazolium glycine	58.39	57.34	1.05	1.80
1-Butyl-3-methylimidazolium hexafluorophosphate	51.46	51.56	-0.10	-0.19
1-Butyl-3-methylimidazolium methosulfate	58.58	58.65	-0.07	-0.12
1-Butyl-3-methylimidazolium octylsulfate	91.49	91.09	0.40	0.44
1-Butyl-3-methylimidazolium perfluorobutylsulfonate	73.34	73.44	-0.10	-0.14
1-Butyl-3-methylimidazolium tetracyanoborate	67.83	67.87	-0.04	-0.06
1-Butyl-3-methylimidazolium tetrafluoroborate	47.81	47.83	-0.02	-0.04
1-Butyl-3-methylimidazolium thiocyanate	57.79	58.09	-0.30	-0.52
1-Butyl-3-methylimidazolium threoninate	68.48	67.95	0.53	0.77
1-Butyl-3-methylimidazolium tricyanomethanide	65.33	65.39	-0.06	-0.09
1-Butyl-3-methylimidazolium trifluoromethylsulfonate	57.91	58.24	-0.33	-0.57
1-Butyl-4-methylpyridinium tetrafluoroborate	54.00	53.84	0.16	0.30
1-Butylpyridinium 2-acryloamido-2-methylpropanesulfonate	91.01	90.15	0.86	0.94
1-Butylpyridinium bis(fluorosulfonyl) amide	64.60	64.65	-0.05	-0.08
1-Butylpyridinium dicyanamide	58.87	58.81	0.06	0.10
1-Butylpyridinium tetrafluoroborate	48.99	49.03	-0.04	-0.08
1-Butyltetrahydrothiophenium dicyanamide	59.59	59.81	-0.22	-0.37
1-Decyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	102.90	102.83	0.07	0.07
1-Decyl-3-methylimidazolium tetracyanoborate	95.66	95.65	0.01	0.01
1-Decyl-3-methylimidazolium tricyanomethanide	93.23	93.17	0.06	0.06
1-Dodecyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	112.08	112.09	-0.01	-0.01
1-Ethyl-2,3-dimethylimidazolium bis(trifluoromethanesulfonyl) amide	69.94	70.13	-0.19	-0.27
1-Ethyl-3-methylimidazolium 1,1,2,2-tetrafluoroethanesulfonate	53.91	53.77	0.14	0.26
1-Ethyl-3-methylimidazolium acetate	44.95	44.65	0.30	0.67

1-Ethyl-3-methylimidazolium aminoacetate	47.68	48.08	-0.40	-0.84
1-Ethyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	65.77	65.79	-0.02	-0.03
1-Ethyl-3-methylimidazolium dicyanamide	48.35	48.35	0.00	0.00
1-Ethyl-3-methylimidazolium diethylphosphate	64.56	64.35	0.21	0.33
1-Ethyl-3-methylimidazolium dimethylphosphate	55.17	55.03	0.14	0.25
1-Ethyl-3-methylimidazolium ethosulfate	54.16	54.05	0.11	0.20
1-Ethyl-3-methylimidazolium imidodisulfonyl fluoride	54.05	54.19	-0.14	-0.26
1-Ethyl-3-methylimidazolium L-alanine	52.10	52.64	-0.54	-1.04
1-Ethyl-3-methylimidazolium L-proline	58.84	59.70	-0.86	-1.46
1-Ethyl-3-methylimidazolium L-serine	54.05	54.05	0.00	0.00
1-Ethyl-3-methylimidazolium methanesulfonate	48.45	48.69	-0.24	-0.50
1-Ethyl-3-methylimidazolium methylsulfate	48.62	49.39	-0.77	-1.58
1-Ethyl-3-methylimidazolium taurinate	56.41	56.96	-0.55	-0.98
1-Ethyl-3-methylimidazolium tetracyanoborate	58.77	58.61	0.16	0.27
1-Ethyl-3-methylimidazolium tetrafluoroborate	38.70	38.57	0.13	0.34
1-Ethyl-3-methylimidazolium thiocyanate	48.31	48.83	-0.52	-1.08
1-Ethyl-3-methylimidazolium threoninate	58.86	58.69	0.17	0.29
1-Ethyl-3-methylimidazolium tricyanomethide	55.87	56.13	-0.26	-0.47
1-Ethyl-3-methylimidazolium trifluoromethylsulfonate	48.91	48.98	-0.07	-0.14
1-Ethyl-3-methylpyridinium bis(fluorosulfonyl) amide	60.16	60.20	-0.04	-0.07
1-Ethyl-3-methylpyridinium ethylsulfate	60.18	60.06	0.12	0.20
1-Ethyl-3-propylimidazolium bis(trifluoromethanesulfonyl) amide	74.95	75.01	-0.06	-0.08
1-Ethylmorpholinium tetrafluoroborate	40.81	39.89	0.92	2.25
1-Ethylpyridinium bis(fluorosulfonyl) amide	55.18	55.39	-0.21	-0.38
1-Ethylpyridinium ethylsulfate	55.29	55.25	0.04	0.07
1-Ethylpyridinium triflate	50.05	50.18	-0.13	-0.26
1-Ethyltetrahydrothiophenium dicyanamide	50.87	50.55	0.32	0.63
1-Heptyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	88.14	88.94	-0.80	-0.91
1-Heptyl-3-methylimidazolium hexafluorophosphate	65.44	65.45	-0.01	-0.02
1-Hexyl-1-methylpyrrolidinium bis(trifluoromethanesulfonyl) amide	87.26	86.13	1.13	1.29
1-Hexyl-3,5-dimethylpyridinium bis(trifluoromethylsulfonyl)amide	95.56	95.13	0.43	0.45

1-Hexyl-3-methylimidazolium acetate	63.54	63.17	0.37	0.58
1-Hexyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	84.23	84.31	-0.08	-0.09
1-Hexyl-3-methylimidazolium chloride	58.80	58.50	0.30	0.51
1-Hexyl-3-methylimidazolium dicyanoamide	67.19	66.87	0.32	0.48
1-Hexyl-3-methylimidazolium hexafluorophosphate	60.69	60.82	-0.13	-0.21
1-Hexyl-3-methylimidazolium tetracyanoborate	76.88	77.13	-0.25	-0.33
1-Hexyl-3-methylimidazolium tetrafluoroborate	56.91	57.09	-0.18	-0.32
1-Hexyl-3-methylimidazolium thiocyanate	68.17	67.35	0.82	1.20
1-Hexyl-3-methylimidazolium tricyanomethanide	74.67	74.65	0.02	0.03
1-Hexylpyridinium bis(fluorosulfonyl) amide	73.94	73.91	0.03	0.04
1-Isobutyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide	77.02	76.83	0.19	0.25
1-Isobutyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	74.92	75.01	-0.09	-0.12
1-Isobutyl-3-methylpyridinium bis(trifluoromethylsulfonyl)amide	81.23	81.02	0.21	0.26
1-Methyl-1-(2',3'-epoxypropyl)-2-oxopyrrolidinium chloride	49.38	49.79	-0.41	-0.83
1-Methyl-1-decylpyrrolidinium bis(trifluoromethanesulfonyl) amide	104.90	104.65	0.25	0.24
1-Methyl-1-propylpiperidinium bis(trifluoromethylsulfonyl)amide	76.90	76.87	0.03	0.04
1-Methyl-1-propylpyrrolidinium bis(fluorosulfonyl) amide	61.04	60.64	0.40	0.66
1-Methyl-1-propylpyrrolidinium bis(trifluoromethanesulfonyl) amide	72.50	72.24	0.26	0.36
1-Methyl-2-pyrrolidonium tetrafluoroborate	37.04	37.68	-0.64	-1.73
1-Methyl-3-hexylimidazolium threoninate	77.73	77.21	0.52	0.67
1-Methyl-3-pentylimidazolium threoninate	73.07	72.58	0.49	0.67
1-Methyl-3-propylimidazolium threoninate	63.75	63.32	0.43	0.67
1-Methylmorpholinium tetrafluoroborate	35.90	35.57	0.33	0.92
1-Methylpiperidinium tetrafluoroborate	37.84	38.51	-0.67	-1.77
1-Methylpyridinium methylsulfate	46.05	46.27	-0.22	-0.48
1-Methylpyrrolidinium tetrafluoroborate	34.55	33.88	0.67	1.94
1-Nonyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	98.06	98.20	-0.14	-0.14
1-Nonyl-3-methylimidazolium hexafluorophosphate	74.74	74.71	0.03	0.04
1-Octyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	93.61	93.57	0.04	0.04

1-Octyl-3-methylimidazolium chloride	67.80	67.76	0.04	0.06
1-Octyl-3-methylimidazolium hexafluorophosphate	70.30	70.08	0.22	0.31
1-Octyl-3-methylimidazolium tetracyanoborate	86.41	86.39	0.02	0.02
1-Octyl-3-methylimidazolium tetrafluoroborate	66.24	66.35	-0.11	-0.17
1-Octyl-3-methylimidazolium tricyanomethanide	84.09	83.91	0.18	0.21
1-Octyl-3-methylpyridinium tetrafluoroborate	72.74	72.36	0.38	0.52
1-Octylpyridinium bis(trifluoromethylsulfonyl)amide	95.19	94.77	0.42	0.44
1-Pentyl-3-methylimidazolium acetate	59.01	58.54	0.47	0.80
1-Pentyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	79.57	79.68	-0.11	-0.14
1-Pentyl-3-methylimidazolium hexafluorophosphate	56.11	56.19	-0.08	-0.14
1-Pentyl-3-methylimidazolium tetrafluoroborate	52.25	52.46	-0.21	-0.40
1-Pentylpyridinium dicyanamide	63.44	63.44	0.00	0.00
1-Phenyl-2,3,5-trimethylpyrazolium methylsulfonate	68.77	69.35	-0.58	-0.84
1-Phenyl-2-butyl-3,5-dimethylpyrazolium methylsulfonate	82.67	82.93	-0.26	-0.31
1-Phenyl-2-heptyl-3,5-dimethylpyrazolium methylsulfonate	97.61	96.82	0.79	0.81
1-Phenyl-2-hexyl-3,5-dimethylpyrazolium methylsulfonate	92.64	92.19	0.45	0.49
1-Phenyl-2-pentyl-3,5-dimethylpyrazolium methylsulfonate	87.17	87.56	-0.39	-0.45
1-Propyl-3-methylimidazolium acetate	49.37	49.28	0.09	0.18
1-Propyl-3-methylimidazolium bis(trifluoromethanesulfonyl) amide	70.48	70.42	0.06	0.09
1-Propyl-3-methylimidazolium tetrafluoroborate	43.09	43.20	-0.11	-0.26
1-Propylpyridinium dicyanamide	54.24	54.18	0.06	0.11
1-Propylpyridinium tetrafluoroborate	44.35	44.40	-0.05	-0.11
1-Propyronitrile-3-butylimidazolium bromide	62.60	62.36	0.24	0.38
1-Propyronitrile-3-hexylimidazolium bromide	71.74	71.62	0.12	0.17
1-Propyronitrile-3-octylimidazolium bromide	80.51	80.88	-0.37	-0.46
2-Hydroxyethylammonium acetate	29.31	28.99	0.32	1.09
2-hydroxyethylammonium butanoate	38.53	38.25	0.28	0.73
2-Hydroxyethylammonium formate	24.85	24.70	0.15	0.60
2-Hydroxyethylammonium hexanoate	47.80	47.51	0.29	0.61
2-Hydroxyethylammonium lactate	34.69	35.04	-0.35	-1.01

2-Hydroxyethylammonium pentanoate	43.12	42.88	0.24	0.56
2-Hydroxyethylammonium propionate	33.29	33.62	-0.33	-0.99
3-Methyl-1-propylpyridinium bis(trifluoromethylsulfonyl)amide	76.40	76.43	-0.03	-0.04
Bis(2-hydroxyethyl)ammonium hexanoate	58.49	58.34	0.15	0.26
Butylammonium nitrate	33.34	33.37	-0.03	-0.09
Dimethyl butyl isopropylammonium bis(trifluoromethylsulfonyl)amide	78.81	79.06	-0.25	-0.32
Dimethyl hexyl isopropylammonium bis(trifluoromethylsulfonyl)amide	89.14	88.32	0.82	0.92
Dimethylpropylisopropylammonium bis(trifluoromethylsulfonyl)amide	73.56	74.43	-0.87	-1.18
Ethylammonium nitrate	24.14	24.11	0.03	0.12
L-Alanine 1-methylethyl ester dodecyl sulfate	102.88	103.30	-0.42	-0.41
L-Alanine 2-methylpropyl ester dodecyl sulfate	107.40	107.88	-0.48	-0.45
L-Proline 1-methylethyl ester dodecyl sulfate	110.32	110.58	-0.26	-0.24
L-Valine 1-methylethyl ester dodecyl sulfate	112.65	112.52	0.13	0.12
Morpholinium formate	32.20	32.26	-0.06	-0.19
N-(2',3'-Epoxypropyl)-N-methylpyrrolidonium acetate	55.50	54.46	1.04	1.87
N-Butyl-3-methylpyridinium bis(trifluoromethylsulfonyl)amide	80.49	81.06	-0.57	-0.71
N-Butyl-3-methylpyridinium trifluoromethanesulfonate	64.26	64.25	0.01	0.02
N-Butyl-4-methylthiazolium bis(trifluoromethylsulfonyl) amide	78.68	79.25	-0.57	-0.72
N-Butyl-4-methylthiazolium difluoro(oxalato)borate	63.24	63.32	-0.08	-0.13
N-Butyl-N-methylmorpholinium N-acetylalaninate	74.32	74.63	-0.31	-0.42
N-Butyl-N-methylmorpholinium N-acetylleucinate	88.43	88.48	-0.05	-0.06
N-Butyl-N-methylmorpholinium N-acetylvalinate	83.98	83.85	0.13	0.15
N-Butylpyridinium bis(trifluoromethanesulfonyl) amide	76.22	76.25	-0.03	-0.04
N-Butylpyridinium triflate	59.25	59.44	-0.19	-0.32
N-Butylpyridinium trifluoroacetate	54.87	55.39	-0.52	-0.95
N-Butylthiazolium bis(trifluoromethylsulfonyl) amide	73.89	74.63	-0.74	-1.00
N-Butylthiazolium difluoro(oxalato)borate	58.43	58.70	-0.27	-0.46
N-Decylpyridinium bis(trifluoromethanesulfonyl) amide	104.52	104.03	0.49	0.47

N-Dodecylpyridinium bis(trifluoromethanesulfonyl) amide	113.68	113.29	0.39	0.34
N-Ethyl-2-methylpyridinium bis(trifluoromethylsulfonyl)amide	71.54	71.54	0.00	0.00
N-Ethylmorpholinium formate	41.07	41.68	-0.61	-1.49
N-Ethyl-N-methylmorpholinium N-acetylalaninate	65.23	65.37	-0.14	-0.21
N-Ethyl-N-methylmorpholinium N-acetylisoleucinate	78.62	79.22	-0.60	-0.76
N-Ethyl-N-methylmorpholinium N-acetylleucinate	78.65	79.22	-0.57	-0.72
N-Ethyl-N-methylmorpholinium N-acetylvalinate	74.01	74.59	-0.58	-0.78
N-Hexyl-N-methylmorpholinium N-acetylalaninate	83.42	83.89	-0.47	-0.56
N-Hexyl-N-methylmorpholinium N-acetylleucinate	97.24	97.74	-0.50	-0.51
N-Hexyl-N-methylmorpholinium N-acetylvalinate	92.26	93.11	-0.85	-0.92
N-Isobutyl-3-sulfopropan-1-aminium hydrogen sulfate	62.85	62.71	0.14	0.22
N-Methyl-N-(2,3-dihydroxypropyl)pyrrolidinium bis(trifluoromethanesulfonyl) amide	74.88	75.07	-0.19	-0.25
N-Octyl-N-methylmorpholinium N-acetylalaninate	92.82	93.15	-0.33	-0.36
N-Octyl-N-methylmorpholinium N-acetylvalinate	102.12	102.37	-0.25	-0.24
N-Propyl-2-methylpyridinium bis(trifluoromethylsulfonyl)amide	76.28	76.17	0.11	0.14
N-Propyl-N-methylmorpholinium N-acetylalaninate	69.57	70.00	-0.43	-0.62
N-Propyl-N-methylmorpholinium N-acetylleucinate	83.88	83.85	0.03	0.04
N-Propyl-N-methylmorpholinium N-acetylvalinate	79.02	79.22	-0.20	-0.25
Propylammonium nitrate	28.78	28.74	0.04	0.14
S-Butyl-dimethylthioformamidium bis(trifluoromethylsulfonyl) amide	79.26	79.02	0.24	0.30
S-Butyl-dimethylthioformamidium difluorooxalylborate	63.42	63.09	0.33	0.52
S-Ethyl-dimethylthioformamidium bis(trifluoromethylsulfonyl) amide	69.84	69.76	0.08	0.11
S-Ethyl-dimethylthioformamidium difluorooxalylborate	53.86	53.83	0.03	0.06

S-Ethyl-dimethylthioformamidium trifluoromethylsulfonate	53.62	52.95	0.67	1.25
S-Methyl-dimethylthioformamidium bis(trifluoromethylsulfonyl) amide	64.95	64.92	0.03	0.05
S-Methyl-dimethylthioformamidium trifluoromethylsulfonate	48.32	48.11	0.21	0.43
Tetrabutylphosphonium acetate	97.22	97.33	-0.11	-0.11
Tetrabutylphosphonium formate	93.57	93.04	0.53	0.57
Tetrabutylphosphonium propanoate	102.16	101.96	0.20	0.20
Tetradecyl trihexylphosphonium bis(trifluoromethylsulfonyl)amide	192.57	192.55	0.02	0.01
Tetradecyl trihexylphosphonium chloride	166.32	166.74	-0.42	-0.25
Tributylmethylammonium bis(trifluoromethylsulfonyl)amide	97.59	97.53	0.06	0.06
Triethylammonium acetate	46.76	46.42	0.34	0.73
Triethyldecylammonium bis(trifluoromethylsulfonyl) amide	111.38	111.11	0.27	0.24
Triethyldodecylammonium bis(trifluoromethylsulfonyl) amide	120.72	120.37	0.35	0.29
Triethylheptylammonium bis(trifluoromethylsulfonyl) amide	97.05	97.22	-0.17	-0.18
Triethylhexylammonium bis(trifluoromethylsulfonyl) amide	92.72	92.59	0.13	0.14
Triethyloctylammonium bis(trifluoromethylsulfonyl) amide	101.96	101.85	0.11	0.11
Triethylsulfonium bis(trifluoromethylsulfonyl) amide	70.04	70.13	-0.09	-0.13
Triethyltetradecylammonium bis(trifluoromethylsulfonyl) amide	129.84	129.63	0.21	0.16
Trihexyl tetradecyl phosphonium dicyanamide	174.84	175.11	-0.27	-0.15
Trihexyl tetradecyl phosphonium trifluoromethylsulfonate	175.69	175.74	-0.05	-0.03
Trimethyl butylammonium bis(trifluoromethylsulfonyl)amide	70.29	70.37	-0.08	-0.11
Trimethyl hexylammonium bis(trifluoromethylsulfonyl)amide	79.64	79.63	0.01	0.01
Trimethyl octylammonium bis(trifluoromethylsulfonyl)amide	88.97	88.89	0.08	0.09
Trimethyl pentylammonium bis(trifluoromethylsulfonyl)amide	75.01	75.00	0.01	0.01
Trimethyl propylammonium bis(trifluoromethylsulfonyl)amide	65.65	65.74	-0.09	-0.14

4.1.2. Silanes, Silanols, Siloxanes, Silazanes and Silicates

Silicon-containing compounds have found use in synthetic processes as intermediates as well as in commercial products, e. g. in detergents, cosmetics, deodorants, soaps, as water-resistant coatings, as defoaming agents or as coolants. Despite the large variety of applications the number of physico-chemical data for this class of molecules is fairly limited within the chemical realm. Nevertheless, a thorough scan of the literature of the last ca. 80 years delivered a sufficient number of data to enable the creation of a basis for the prediction of several chemical descriptors of interest based on the present atom-group additivity principle. Accordingly, in analogy to the previous section, the updated parameters tables provided the group parameters for the heat of combustion [403], enabling its calculation for 99 silicon compounds with a correlation coefficient R^2 of 1.0 and a MAPD of 0.19%, for the heat of vaporization [404] for 103 ($R^2=0.8164$, MAPD=10.31%), for the surface tension [405] of 18 ($R^2=0.9834$, MAPD=2.62%), for the liquid heat capacity at 293K [376] of 26 ($R^2=0.9981$, MAPD=2.32%), for the solid heat capacity at 293K [406] of 14 ($R^2=0.9925$, MAPD=2.77%), for the standard entropy of fusion [404] of 45 ($R^2=0.7251$, MAPD=15.09%), and even for the vapour pressure [407] of 9 silicon compounds ($R^2=0.9897$, MAPD=7.92%). In addition to these descriptors, the present work now provides the refractivity data for 351 silicon derivatives, alphabetically sampled in Table 5. They prove the reliability of the calculated values with a MAPD of only 0.39%, compared with their experimental values.

Table 5. Calculated and experimental refractivity of silicon-containing compounds

Molecule name	Refractivity exp	Refractivity calc	Deviation	Dev. in %
(2-Phenylethyl)trichlorosilane	58.62	58.57	0.05	0.09
(3-Chloropropyl)trichlorosilane	43.26	43.44	-0.18	-0.42
(3-Chloropropyl)trimethoxysilane	46.53	46.62	-0.09	-0.19
(3-Chloropropyl)trimethylsilane	44.47	44.33	0.14	0.31
(4-Bromophenoxy)trimethylsilane	58.55	58.44	0.11	0.19
(4-Chlorophenyl)trichlorosilane	55.04	54.14	0.90	1.64
(4-Methoxyphenyl)trimethylsilane	56.94	56.73	0.21	0.37
(4-Methylphenyl)trimethylsilane	54.82	55.02	-0.20	-0.36
(Bromomethyl)chlorodimethylsilane	37.57	37.57	0.00	0.00
(Bromomethyl)trimethylsilane	38.09	38.08	0.01	0.03
(Chloromethyl)trichlorosilane	34.10	34.12	-0.02	-0.06
(Chloromethyl)trimethylsilane	35.13	35.01	0.12	0.34
(Dichloromethyl)trichlorosilane	39.36	39.06	0.30	0.76
(Diethylamino)trimethylsilane	47.33	47.09	0.24	0.51
1,1,1,3,5,5,5-Heptamethyltrisiloxane	63.17	63.24	-0.07	-0.11
1,1,1,3,5,7,7,7-Octamethyltetrasiloxane	77.46	77.53	-0.07	-0.09
1,1,3,3-Tetramethyl-1,3-diphenyldisiloxane	88.87	88.71	0.16	0.18
1,1,3,3-Tetramethyldisiloxane	40.19	40.23	-0.04	-0.10
1,2-Bis(tributylsilyl)acetylene	138.06	138.22	-0.16	-0.12
1,2-Bis(triethylsilyl)ethane	85.59	85.82	-0.23	-0.27
1,2-Bis(trimethylsilyl)acetylene	55.18	55.24	-0.06	-0.11
1,2-Dis(trimethylsilyl)-ethylene	58.50	58.06	0.44	0.75

1,3,5-Trisilacyclohexane	43.69	43.44	0.25	0.57
1,3-Bis(bromomethyl)tetramethyldisiloxane	64.41	64.45	-0.04	-0.06
1,3-Bis(chloromethyl)tetramethyldisiloxane	58.30	58.31	-0.01	-0.02
1,3-Bis(dichloromethyl)tetramethyldisiloxane	68.07	68.19	-0.12	-0.18
1,3-Bis(trimethylsiloxy)benzene	75.39	75.18	0.21	0.28
1,3-Divinyl-1,1,3,3-tetramethyldisiloxane	57.23	57.33	-0.10	-0.17
1-Heptyltrifluorosilane	41.32	41.07	0.25	0.61
2,2,4,4,6,6-Hexamethylcyclotrisilazane	63.90	63.78	0.12	0.19
2,4,6,8,10,12-Hexamethylcyclohexasiloxane	85.86	85.74	0.12	0.14
2,4,6,8-Tetramethylcyclotetrasiloxane	57.13	57.16	-0.03	-0.05
2,4,6-Trimethyl-2,4,6-triphenylcyclotrisiloxane	115.86	115.59	0.27	0.23
2-Butylsilane	31.02	31.09	-0.07	-0.23
2-Pentyloxytrimethylsilane	49.75	49.57	0.18	0.36
2-Silylpentasilane	73.17	73.09	0.08	0.11
2-Silyltetrasilane	61.12	61.05	0.07	0.11
2-Silyltrisilane	48.88	49.01	-0.13	-0.27
3-(Triethoxysilyl)-1-propanamine	59.24	59.23	0.01	0.02
3-(Trimethylsilyl)-1-propanol	41.55	40.94	0.61	1.47
3-Mercaptopropyl-trimethoxysilane	49.46	49.49	-0.03	-0.06
4-Bromophenyltrimethylsilane	57.19	57.80	-0.61	-1.07
4-Chlorophenoxytriethylsilane	69.66	69.38	0.28	0.40
4-Fluorophenyltrimethylsilane	50.34	50.11	0.23	0.46
4-Trifluoromethylphenyltrimethylsilane	54.63	55.30	-0.67	-1.23
4-Trimethylsiloxyphenyltrimethylsilane	74.63	74.54	0.09	0.12
Allylchlorodimethylsilane	37.98	38.71	-0.73	-1.92
Allylmethyldichlorosilane	38.14	38.50	-0.36	-0.94
Allyltrichlorosilane	38.97	38.33	0.64	1.64
Allyltriethoxysilane	55.73	55.49	0.24	0.43
Allyltrimethylsilane	39.14	39.22	-0.08	-0.20
Amylsilane	35.64	35.67	-0.03	-0.08
Benzyltrimethylsilane	55.11	54.83	0.28	0.51
Bis(butylthio) 2-(diethylmethylsilyl)ethyl borane	101.77	102.28	-0.51	-0.50
Bis(diethyl)disiloxane	58.54	58.51	0.03	0.05
Bis(diethylmethylsilyl)amine	69.24	69.58	-0.34	-0.49
Bis(diethylsilyl)amine	61.40	61.24	0.16	0.26
Bis(dimethylamino)bis(diethylamino)silane	79.50	79.36	0.14	0.18
Bis(dimethylphenylsilyl)amine	91.08	91.06	0.02	0.02
Bis(ethyldimethylsilyl)amine	61.01	60.44	0.57	0.93
Bis(ethylisobutyl)disiloxane	76.95	76.95	0.00	0.00
Bis(ethylphenyl)disiloxane	88.84	89.13	-0.29	-0.33
Bis(trichlorosilyl)methane	51.08	51.72	-0.64	-1.25

Bis(triethylsilyl)amine	78.33	78.72	-0.39	-0.50
Bis(trihexylsilyl)acetylene	193.90	193.78	0.12	0.06
Bis(trimethoxysilyl)amine	56.30	56.38	-0.08	-0.14
Bis(trimethoxysilylamino)dimethylsilane	77.61	77.64	-0.03	-0.04
Bis(trimethylsilylamino)dimethylsilane	71.81	72.56	-0.75	-1.04
Bromotriethylsilane	46.44	46.60	-0.16	-0.34
Bromotrimethylsilane	32.92	32.89	0.03	0.09
Butoxytrimethylsilane	44.88	44.93	-0.05	-0.11
Butylsilane	30.90	31.04	-0.14	-0.45
Butyltrichlorosilane	43.18	43.27	-0.09	-0.21
Butyltriisothiocyanatosilane	73.92	73.73	0.19	0.26
Chloro(chloromethyl)dimethylsilane	34.43	34.50	-0.07	-0.20
Chloro(dichloromethyl)dimethylsilane	39.39	39.44	-0.05	-0.13
Chlorodiethylsilane	34.92	34.70	0.22	0.63
Chlorodimethylphenylsilane	49.33	49.70	-0.37	-0.75
Chlorodimethylsilane	25.90	25.56	0.34	1.31
Chloroethyldimethylsilane	35.15	34.39	0.76	2.16
Chloromethylphenylsilane	45.46	45.44	0.02	0.04
Chlorotriethylsilane	43.54	43.53	0.01	0.02
Chlorotrimethylsilane	29.88	29.82	0.06	0.20
Chlorovinyl dimethylsilane	34.49	34.01	0.48	1.39
cis-1,2-Bis(trimethylsilyl)-3,3-dichlorocyclopropane	71.37	70.62	0.75	1.05
cis-1,2-Dis(trimethylsilyl)-ethylene	57.88	58.06	-0.18	-0.31
Cyclohexyloxytrimethylsilane	52.12	52.06	0.06	0.12
Cyclohexyltrifluorosilane	34.26	34.35	-0.09	-0.26
Decamethylcyclopentasiloxane	93.33	93.25	0.08	0.09
Decamethyltetrasiloxane	86.18	86.25	-0.07	-0.08
Decyldiphenylnonylsilane	148.69	148.68	0.01	0.01
Decyldiphenylsilane	106.74	107.04	-0.30	-0.28
Decyloxytrimethylsilane	72.71	72.71	0.00	0.00
Di(cyclohexyloxy)dimethylsilane	74.01	73.82	0.19	0.26
Diallyldimethylsilane	48.34	48.11	0.23	0.48
Diamylsilane	58.60	58.56	0.04	0.07
Dibutyl-diisothiocyanatosilane	77.77	77.84	-0.07	-0.09
Dibutyl dinonylsilane	131.54	131.95	-0.41	-0.31
Dibutylmethylsilyl bromide	60.64	60.55	0.09	0.15
Dibutyl nonylsilane	90.16	90.31	-0.15	-0.17
Dibutylsilane	49.39	49.30	0.09	0.18
Dichloro(chloromethyl)methylsilane	34.17	34.29	-0.12	-0.35
Dichloro(dichloromethyl)methylsilane	39.13	39.23	-0.10	-0.26
Dichlorodiethylsilane	38.71	38.75	-0.04	-0.10

Dichlorodimethylsilane	29.65	29.61	0.04	0.13
Dichlorodiphenylsilane	69.99	69.37	0.62	0.89
Dichloromethylphenylsilane	48.81	49.49	-0.68	-1.39
Dicosamethyldecasiloxane	197.51	198.15	-0.64	-0.32
Didecyldiphenylsilane	153.40	153.31	0.09	0.06
Diethoxydimethylsilane	40.99	41.04	-0.05	-0.12
Diethoxydiphenylsilane	81.07	80.80	0.27	0.33
Diethoxymethylphenylsilane	60.85	60.92	-0.07	-0.12
Diethoxymethylsilane	36.84	36.68	0.16	0.43
Diethyl 2,2-diethylhydrazinosilane	55.43	55.86	-0.43	-0.78
Diethyl 2,2-dimethylhydrazinosilane	46.39	46.68	-0.29	-0.63
Diethyl bis(2,2-diethylhydrazino)silane	81.18	80.88	0.30	0.37
Diethyl bis(2,2-dimethylhydrazino)silane	62.47	62.52	-0.05	-0.08
Diethyl diethylaminosilane	52.34	52.06	0.28	0.53
Diethyldifluorosilane	27.74	27.83	-0.09	-0.32
Diethyldiisothiocyanatosilane	59.55	59.32	0.23	0.39
Diethylmethylchlorosilane	38.62	38.96	-0.34	-0.88
Diethylmethylsilanol	35.43	35.61	-0.18	-0.51
Diethylnonylsilane	71.60	71.79	-0.19	-0.27
Diethyloctylsilane	67.23	67.16	0.07	0.10
Diethylphenyl 1-isopropoxyethoxysilane	80.26	80.12	0.14	0.17
Diethylsilane	30.71	30.78	-0.07	-0.23
Diethylsilanol	31.62	31.25	0.37	1.17
Difluorodiphenylsilane	58.69	58.45	0.24	0.41
Dimethoxydiphenylsilane	71.70	71.48	0.22	0.31
Dimethyl bis(2,2-diethylhydrazino)silane	71.55	71.74	-0.19	-0.27
Dimethyl bis(2,2-dimethylhydrazino)silane	53.54	53.38	0.16	0.30
Dimethyl bis(2-chloropropoxy)silane	59.83	59.82	0.01	0.02
Dimethyldi(2-ethylbutoxy)silane	78.27	78.00	0.27	0.34
Dimethyldi(2-octyloxy)silane	96.44	96.62	-0.18	-0.19
Dimethyldi-2-butoxysilane	59.68	59.58	0.10	0.17
Dimethyldi-2-pentoxysilane	68.61	68.84	-0.23	-0.34
Dimethyldiacetoxysilane	40.81	40.82	-0.01	-0.02
Dimethyldibutoxysilane	59.63	59.56	0.07	0.12
Dimethyldidodecyloxysilane	133.43	133.64	-0.21	-0.16
Dimethyldiheptoxysilane	87.25	87.34	-0.09	-0.10
Dimethyldihexoxysilane	77.46	78.08	-0.62	-0.80
Dimethyldiisopropoxysilane	49.53	50.32	-0.79	-1.59
Dimethyldiisothiocyanatosilane	49.92	50.18	-0.26	-0.52
Dimethyldimethoxysilane	31.51	31.72	-0.21	-0.67
Dimethyldinonyloxysilane	105.67	105.86	-0.19	-0.18

Dimethyldioctoxysilane	96.50	96.60	-0.10	-0.10
Dimethyldipentoxysilane	68.38	68.82	-0.44	-0.64
Dimethyldiphenoxysilane	71.56	71.40	0.16	0.22
Dimethyldiphenylsilane	70.04	70.09	-0.05	-0.07
Dimethyldipropoxysilane	50.94	50.30	0.64	1.26
Dimethylethylsilanol	30.79	31.04	-0.25	-0.81
Dimethylphenylsilane	45.04	45.55	-0.51	-1.13
Dimethylvinylethoxysilane	39.82	39.86	-0.04	-0.10
Dinonyldiphenylsilane	144.50	144.05	0.45	0.31
Diphenylmethylsilane	65.28	65.43	-0.15	-0.23
Diphenylmethylsilylamine	68.03	68.05	-0.02	-0.03
Diphenylnonylsilane	102.30	102.41	-0.11	-0.11
Diphenylsilane	61.53	61.40	0.13	0.21
Dipropyldifluorosilane	37.24	37.09	0.15	0.40
Dipropylsilane	40.08	40.04	0.04	0.10
Disilanomethane	27.16	27.26	-0.10	-0.37
Dodecamethylcyclohexasiloxane	111.89	111.90	-0.01	-0.01
Dodecamethylpentasiloxane	104.79	104.90	-0.11	-0.10
Eicosamethylnonasiloxane	179.30	179.50	-0.20	-0.11
Ethoxytriethylsilane	49.10	49.38	-0.28	-0.57
Ethoxytrihexylsilane	105.58	104.94	0.64	0.61
Ethoxytrimethylsilane	35.67	35.67	0.00	0.00
Ethyl bis(2,2-diethylhydrazino)silane	71.76	71.89	-0.13	-0.18
Ethyl bis(2,2-dimethylhydrazino)silane	53.67	53.53	0.14	0.26
Ethyl bis(2-chloropropoxy)silane	59.73	60.03	-0.30	-0.50
Ethyl bis(diethylamino)silane	64.26	64.29	-0.03	-0.05
Ethyl isobutyl 2-chloropropoxysilane	59.24	59.06	0.18	0.30
Ethyl tris(2,2-diethylhydrazino)silane	96.93	96.81	0.12	0.12
Ethylaminotriethylsilane	51.46	51.36	0.10	0.19
Ethylcyclohexyldifluorosilane	44.31	44.26	0.05	0.11
Ethyl dibutoxysilane	59.63	59.77	-0.14	-0.23
Ethyl dimethyl 1-(3-pentoxo)ethoxysilane	64.89	64.93	-0.04	-0.06
Ethylisobutylsilanol	40.40	40.47	-0.07	-0.17
Ethylphenylchlorosilane	49.44	50.01	-0.57	-1.15
Ethyltributoxysilane	78.67	78.95	-0.28	-0.36
Ethyltrichlorosilane	33.83	34.01	-0.18	-0.53
Ethyltriethoxysilane	51.50	51.17	0.33	0.64
Ethyltriisothiocyantosilane	64.17	64.47	-0.30	-0.47
Ethyltrimethoxysilane	37.01	37.19	-0.18	-0.49
Fluoroethyldiisopropylsilane	47.71	47.87	-0.16	-0.34
Fluorotributylsilane	66.71	66.29	0.42	0.63

Fluorotriethylsilane	38.10	38.51	-0.41	-1.08
Fluorotripentylsilane	80.30	80.18	0.12	0.15
Fluorotripropylsilane	52.33	52.40	-0.07	-0.13
Heptasilane	84.77	84.84	-0.07	-0.08
Heptyloxytrimethylsilane	58.80	58.82	-0.02	-0.03
Hexadecamethylheptasiloxane	142.31	142.20	0.11	0.08
Hexaethyldisiloxane	75.92	76.37	-0.45	-0.59
Hexamethyldisilane	51.42	51.36	0.06	0.12
Hexamethyldisiloxane	48.94	48.95	-0.01	-0.02
Hexapropyldisiloxane	104.05	104.15	-0.10	-0.10
Hexasilane	72.78	72.80	-0.02	-0.03
Hexyloxytrimethylsilane	54.16	54.19	-0.03	-0.06
Hexylsilane	40.34	40.30	0.04	0.10
HMDS	51.55	51.30	0.25	0.48
iso-Butylsilane	31.05	31.00	0.05	0.16
Isopentyloxytrimethylsilane	49.54	49.52	0.02	0.04
Isopropylmethylsilane	30.66	30.89	-0.23	-0.75
Isopropyltriisothiocyanatosilane	69.52	69.15	0.37	0.53
Isopropyltrimethylsilane	38.47	39.58	-1.11	-2.89
Methoxytriethylsilane	44.49	44.72	-0.23	-0.52
Methoxytrimethylsilane	30.80	31.01	-0.21	-0.68
Methoxytripropylsilane	58.64	58.61	0.03	0.05
Methyl bis(2,2-diethylhydrazino)silane	67.18	67.32	-0.14	-0.21
Methyl bis(2,2-dimethylhydrazino)silane	48.80	48.96	-0.16	-0.33
Methyl bis(2-chloropropoxy)silane	55.37	55.46	-0.09	-0.16
Methyl bis(diethylamino)silane	59.99	59.72	0.27	0.45
Methyl tris(2,2-diethylhydrazino)silane	92.26	92.24	0.02	0.02
Methylcyclohexyldifluorosilane	39.68	39.69	-0.01	-0.03
Methyldibutoxysilane	54.87	55.20	-0.33	-0.60
Methyldichloro-2-(2,4-dichlorophenoxy)ethylsilane	70.31	70.12	0.19	0.27
Methyldichloro-2-(4-chlorophenoxy)ethylsilane	65.49	65.30	0.19	0.29
Methyldichloro-2,4-dichlorophenoxysilane	60.94	60.20	0.74	1.21
Methyldichloro-2-butoxyethylsilane	55.11	54.39	0.72	1.31
Methyldichloro-2-isobutoxyethylsilane	54.52	54.35	0.17	0.31
Methyldichloro-2-phenoxyethylsilane	60.39	60.48	-0.09	-0.15
Methyldichloro-4-chlorophenoxysilane	55.08	55.38	-0.30	-0.54
Methyldichlorobutoxysilane	44.66	44.64	0.02	0.04
Methyldichlorophenoxysilane	50.14	50.56	-0.42	-0.84
Methyldiethyl-2-phenoxyethylsilane	70.07	70.34	-0.27	-0.39
Methyldiethylphenoxysilane	60.29	59.99	0.30	0.50
Methylnonylphenylsilane	82.90	82.53	0.37	0.45

Methyloctylphenylsilane	78.18	77.90	0.28	0.36
Methylphenyldifluorosilane	38.26	38.57	-0.31	-0.81
Methylphenylsilane	40.82	41.52	-0.70	-1.71
Methylpropylsilane	30.73	30.84	-0.11	-0.36
Methylsilanetriol triacetate	46.27	46.27	0.00	0.00
Methyltri(2-octyloxy)silane	129.85	129.97	-0.12	-0.09
Methyltributoxysilane	74.39	74.38	0.01	0.01
Methyltrichlorosilane	29.13	29.44	-0.31	-1.06
Methyltriheptyloxysilane	116.01	116.05	-0.04	-0.03
Methyltrihexyloxysilane	102.11	102.16	-0.05	-0.05
Methyltriisopentyloxysilane	88.26	88.15	0.11	0.12
Methyltripentyloxysilane	88.20	88.27	-0.07	-0.08
Methyltriphenoxysilane	91.85	92.14	-0.29	-0.32
Methylvinylchlorosilane	33.33	33.80	-0.47	-1.41
N-(1,1-Dimethylpropyl)aminotriethylsilane	64.79	65.18	-0.39	-0.60
N-(3-(Trimethoxysilyl)propyl)-1,2-ethanediamine	58.21	57.88	0.33	0.57
N,N-Dibutylaminotriethylsilane	78.65	79.32	-0.67	-0.85
N,N-Diethylaminotriethylsilane	60.99	60.80	0.19	0.31
N,N-Diisobutylaminotriethylsilane	78.67	79.24	-0.57	-0.72
N-Fenchylaminotriethylsilane	83.74	83.97	-0.23	-0.27
N-Isopropylaminotriethylsilane	56.05	55.92	0.13	0.23
Nonyloxytrimethylsilane	68.07	68.08	-0.01	-0.01
N-Propylaminotriethylsilane	56.11	55.99	0.12	0.21
N-t-Butylaminotriethylsilane	60.63	60.55	0.08	0.13
Octadecamethyloctasiloxane	160.19	160.85	-0.66	-0.41
Octadecyltrichlorosilane	108.02	108.09	-0.07	-0.06
Octamethylcyclotetrasiloxane	74.68	74.60	0.08	0.11
Octamethyltrisiloxane	67.44	67.60	-0.16	-0.24
Octyloxytrimethylsilane	63.43	63.45	-0.02	-0.03
Pentasilane	60.80	60.76	0.04	0.07
Pentyloxytrimethylsilane	49.52	49.56	-0.04	-0.08
Pentyltrichlorosilane	48.79	47.90	0.89	1.82
Phenoxytriethylsilane	64.47	64.56	-0.09	-0.14
Phenoxytrimethylsilane	51.17	50.85	0.32	0.63
Phenoxytripropylsilane	78.41	78.45	-0.04	-0.05
Phenylsilane	37.44	37.09	0.35	0.93
Phenyltri(2-octyloxy)silane	149.82	149.85	-0.03	-0.02
Phenyltri(cyclohexyloxy)silane	115.70	115.65	0.05	0.04
Phenyltrichlorosilane	48.92	49.32	-0.40	-0.82
Phenyltrifluorosilane	33.09	33.23	-0.14	-0.42
Phenyltriisopentyloxysilane	108.25	108.03	0.22	0.20

Phenyltrimethylsilane	49.88	50.21	-0.33	-0.66
Propyltrichlorosilane	38.46	38.64	-0.18	-0.47
Propyltriisothiocyanatosilane	68.69	69.10	-0.41	-0.60
t-Butoxytriethylsilane	58.54	58.59	-0.05	-0.09
t-Butoxytrimethylsilane	44.98	44.88	0.10	0.22
t-Butoxytripropylsilane	72.68	72.48	0.20	0.28
Tetra(1H,1H,3H-perfluoropropyl)silicate	72.19	72.10	0.09	0.12
Tetra(1H,1H,5H-perfluoropentyl)silicate	111.97	112.18	-0.21	-0.19
Tetra(2-ethylbutyl) silicate	125.53	126.42	-0.89	-0.71
Tetra(diethylamino)silane	97.33	97.72	-0.39	-0.40
Tetra(dimethylamino)silane	61.29	61.00	0.29	0.47
Tetra-2-butoxysilane	90.48	89.58	0.90	0.99
Tetra-2-methyl-1-propoxysilane	88.88	89.38	-0.50	-0.56
Tetra-2-pentoxysilane	108.98	108.10	0.88	0.81
Tetra-3-methyl-1-butoxysilane	107.23	107.90	-0.67	-0.62
Tetrabutoxysilane	88.88	89.54	-0.66	-0.74
Tetracosamethylhendecasiloxane	217.25	216.80	0.45	0.21
Tetradecamethylcycloheptasiloxane	130.84	130.55	0.29	0.22
Tetradecamethylhexasiloxane	123.45	123.55	-0.10	-0.08
Tetraethoxysilane	53.33	52.50	0.83	1.56
Tetraethylsilane	48.37	48.61	-0.24	-0.50
Tetrahexoxysilane	127.50	126.58	0.92	0.72
Tetraisobutylsilane	86.00	85.49	0.51	0.59
Tetraisopropoxysilane	70.82	71.06	-0.24	-0.34
Tetraisopropylsilane	66.92	67.33	-0.41	-0.61
Tetramethylsilane	29.95	30.33	-0.38	-1.27
Tetramethyltetraphenylcyclotetrasiloxane	154.31	154.12	0.19	0.12
Tetramethyoxysilane	33.51	33.86	-0.35	-1.04
Tetraoctoxysilane	163.90	163.62	0.28	0.17
Tetrapentoxysilane	107.38	108.06	-0.68	-0.63
Tetrapropoxysilane	70.65	71.02	-0.37	-0.52
Tetrasilane	48.89	48.72	0.17	0.35
Tetravinylsilane	46.88	47.09	-0.21	-0.45
trans-1,2-Bis(trimethylsilyl)-3,3-dichlorocyclopropane	71.02	70.62	0.40	0.56
Tributylisothiocyanatosilane	82.05	81.60	0.45	0.55
Tributylsilane	67.51	67.16	0.35	0.52
Tributylsilanol	67.79	67.96	-0.17	-0.25
Tributylsilylamine	69.61	69.78	-0.17	-0.24
Trichloro-2-phenoxyethylsilane	60.44	60.31	0.13	0.22
Trichlorovinylsilane	33.54	33.63	-0.09	-0.27
Triethoxymethylsilane	46.50	46.60	-0.10	-0.22

Triethoxypentylsilane	64.96	65.06	-0.10	-0.15
Triethoxyphenylsilane	66.15	66.48	-0.33	-0.50
Triethyl 1-propoxyethoxysilane	65.15	64.80	0.35	0.54
Triethyl 2,2-diethylhydrazinosilane	64.50	64.60	-0.10	-0.16
Triethyl 2,2-dimethylhydrazinosilane	55.48	55.42	0.06	0.11
Triethylisothiocyanatosilane	53.85	53.82	0.03	0.06
Triethylsilane	39.60	39.38	0.22	0.56
Triethylsilanol	40.59	40.18	0.41	1.01
Triethylsilylamine	42.07	42.00	0.07	0.17
Triethylsilyloxytripropylsilane	90.19	90.26	-0.07	-0.08
Triethyltriphenylcyclotrisiloxane	129.17	129.30	-0.13	-0.10
Triisopropoxyvinylsilane	65.03	64.71	0.32	0.49
Triisopropylethoxysilane	63.56	63.42	0.14	0.22
Triisopropylphenylsilane	77.50	77.96	-0.46	-0.59
Triisopropylsilane	53.57	53.42	0.15	0.28
Triisopropylsilyl chloride	57.72	57.57	0.15	0.26
Trimethoxymethylsilane	32.24	32.62	-0.38	-1.18
Trimethoxyphenylsilane	52.32	52.50	-0.18	-0.34
Trimethoxysilylamine	30.95	30.83	0.12	0.39
Trimethyl 1-ethoxyethoxysilane	46.52	46.46	0.06	0.13
Trimethyl 1-isopropoxyethoxysilane	51.15	51.10	0.05	0.10
Trimethyl 2,2-diethylhydrazinosilane	50.99	50.89	0.10	0.20
Trimethyl 2,2-dimethylhydrazinosilane	41.77	41.71	0.06	0.14
Trimethylisothiocyanatosilane	40.13	40.11	0.02	0.05
Trimethylsilanol	26.22	26.47	-0.25	-0.95
Trimethylsilylaminodimethylphenylsilane	71.09	71.18	-0.09	-0.13
Trimethylsilylaminodiphenylmethylsilane	91.05	91.06	-0.01	-0.01
Trimethylsilylaminotriethylsilane	65.00	65.01	-0.01	-0.02
Trimethylsilylaminotrimethoxysilane	53.70	53.84	-0.14	-0.26
Trimethylsilylaminotriphenylsilane	111.69	110.94	0.75	0.67
Trimethylsilyloxytriethylsilane	62.45	62.66	-0.21	-0.34
Trimethylsilyloxytripropylsilane	76.55	76.55	0.00	0.00
Trimethylvinylsilane	34.55	34.52	0.03	0.09
Tripentylsilane	81.54	81.05	0.49	0.60
Tripropylsilane	52.75	53.27	-0.52	-0.99
Tris(dimethylamino)dibutylaminosilane	88.58	88.70	-0.12	-0.14
Trisilane	36.61	36.68	-0.07	-0.19
Vinyl tris(2-chloropropoxy)silane	79.31	78.96	0.35	0.44
Vinyldiethoxymethylsilane	45.09	45.23	-0.14	-0.31
Vinyltriacetoxysilane	50.55	50.46	0.09	0.18
Vinyltriethoxysilane	50.75	50.79	-0.04	-0.08

Vinyltrimethoxysilane	36.41	36.81	-0.40	-1.10
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4.1.3. Boranes, Borines, Borazines, Boronates and Borates

In contrast to the prior two sections, boron-containing compounds are essentially important intermediates in chemical syntheses, and therefore experimental physico-chemical data are scarce. The large number of refractivity data, on the other hand, is primarily owed to the need to characterize the newly synthesized molecules by some easily accessible physical data, such as elemental analysis, melting point, density and refractive index. With a few exceptions (e. g. Christopher et al. [80]) however, most authors did not show any interest in using the latter two values for the calculation of the molecules' refractivity or polarizability. The present collection of refractivity data for 137 boron compounds listed in Table 6, although perhaps of merely academic interest, nevertheless confirms - by the strong linearity over the complete set - the overall correctness of the experimental data and at the same time proves the versatility of the present group-additivity approach, revealing a MAPD of just 0.46%.

Table 6. Calculated and experimental refractivity of boron-containing compounds

Molecule name	Refractivity exp	Refractivity calc	Deviation	Dev. in %
1,2-Bis(dipentylborinoxy)ethane	116.12	116.10	0.02	0.02
1,3,5-Tributylborazine	79.59	79.86	-0.27	-0.34
1,3,5-Triethylborazine	52.48	52.08	0.40	0.76
1,3-Bis(dibutoxyboryl)propane	104.73	104.83	-0.10	-0.10
1,3-Bis(dichloroboryl)propane	44.12	44.25	-0.13	-0.29
1,3-Bis(dimethoxyboryl)propane	48.96	49.15	-0.19	-0.39
1,4-Bis(dichloroboryl)butane	48.79	48.88	-0.09	-0.18
1,4-Bis(diethoxyboryl)butane	73.12	72.42	0.70	0.96
1,5-Bis(diethoxyboryl)pentane	77.13	77.05	0.08	0.10
1,6-Bis(diethoxyboryl)hexane	81.81	81.68	0.13	0.16
2-Butoxy-2-bora-1,3-dioxacyclopentane	37.13	36.61	0.52	1.40
2-Tolyl 3-tolyl propoxyborine	82.11	81.86	0.25	0.30
2-Tolyl 4-tolyl propoxyborine	82.26	81.86	0.40	0.49
2-Tolyl dibutoxyborine	76.18	76.43	-0.25	-0.33
2-Tolyl diethoxyborine	57.69	57.91	-0.22	-0.38
2-Tolyl dimethoxyborine	48.14	48.59	-0.45	-0.93
2-Tolyl dipropoxyborine	66.97	67.17	-0.20	-0.30
3-Tolyl dibutoxyborine	76.48	76.43	0.05	0.07
3-Tolyl diethoxyborine	58.08	57.91	0.17	0.29
3-Tolyl dimethoxyborine	48.38	48.59	-0.21	-0.43
3-Tolyl dipropoxyborine	67.26	67.17	0.09	0.13
4-Tolyl dibutoxyborine	76.67	76.43	0.24	0.31
4-Tolyl diethoxyborine	58.04	57.91	0.13	0.22

4-Tolyl dimethoxyborine	48.49	48.59	-0.10	-0.21
4-Tolyl dipropoxyborine	67.42	67.17	0.25	0.37
Bis(2-tolyl)-N-ethylaminoborane	79.12	78.87	0.25	0.32
Bis(2-tolyl)-N-isobutylaminoborane	88.08	88.09	-0.01	-0.01
Bis(2-tolyl)-N-methylaminoborane	74.00	74.28	-0.28	-0.38
Bis(allylamino)borane	40.89	41.33	-0.44	-1.08
Bis(butylamino)borane	51.24	51.21	0.03	0.06
Bis(butylthio) 2-(diethylmethylsilyl)ethyl borane	101.77	102.28	-0.51	-0.50
Bis(butylthio) hexyl borane	88.58	88.16	0.42	0.47
Bis(butylthio) octyl borane	98.30	97.42	0.88	0.90
Bis(butylthio)borane	60.17	60.27	-0.10	-0.17
Bis(diallylamino)borane	67.84	68.71	-0.87	-1.28
Bis(diethylamino)borane	51.54	51.43	0.11	0.21
Bis(di-isoamylamino)borane	107.11	106.83	0.28	0.26
Bis(diisobutylamino)borane	88.26	88.31	-0.05	-0.06
Bis(ethylthio) butylborane	60.19	60.38	-0.19	-0.32
Bis(ethylthio) isobutylborane	60.30	60.34	-0.04	-0.07
Bis(ethylthio) isopropylborane	55.34	55.77	-0.43	-0.78
Bis(ethylthio) octyl borane	78.77	78.90	-0.13	-0.17
Bis(ethylthio) propylborane	55.66	55.75	-0.09	-0.16
Bis(ethylthio)borane	41.16	41.75	-0.59	-1.43
Bis(isobutyl) cyclohexylboronate	72.44	72.12	0.32	0.44
Bis(isopropylthio)borane	51.08	50.99	0.09	0.18
Bis(propylthio)borane	50.77	51.01	-0.24	-0.47
Bis(t-butylthio)borane	61.77	61.01	0.76	1.23
Bromo butylthio isopentylborane	64.00	63.96	0.04	0.06
Bromo ethylthio isopentylborane	54.51	54.70	-0.19	-0.35
Bromo ethylthio isopropylborane	45.04	45.50	-0.46	-1.02
Bromo ethylthio phenylborane	57.27	56.67	0.60	1.05
Butoxy chloro phenylborine	56.56	56.22	0.34	0.60
Butyl butoxy chloroborine	49.43	49.66	-0.23	-0.47
Butyl dibutoxyborine	64.87	65.06	-0.19	-0.29
Butylphenylboronic acid	50.06	50.81	-0.75	-1.50
Butylthiodiethylborane	52.20	52.20	0.00	0.00
Chloro 2-octoxy phenylborine	74.42	74.75	-0.33	-0.44
Chloro di(1,2,2-trimethylpropoxy)borine	69.31	69.36	-0.05	-0.07
Chloro di(2-octoxy)borine	87.34	87.92	-0.58	-0.66
Chloro di(sec-butoxy)borine	50.69	50.88	-0.19	-0.37
Chloro dibutoxyborine	51.03	50.86	0.17	0.33
Chloro diisobutoxyborine	50.35	50.78	-0.43	-0.85
Chloro dineopentoxyborine	60.34	60.08	0.26	0.43

Chloro dioctoxyborine	88.29	87.90	0.39	0.44
Chloro dipropoxyborine	41.83	41.60	0.23	0.55
Cyclohexyldichloroborane	41.98	41.91	0.07	0.17
Dibutoxy 2-hydroxyethoxy borine	59.48	58.68	0.80	1.34
Dibutylboronic anhydride	86.44	87.19	-0.75	-0.87
Dibutylbutylaminoborane	65.68	65.39	0.29	0.44
Dibutylethylthioborane	61.49	61.46	0.03	0.05
Dibutylphenylaminoborane	72.53	72.57	-0.04	-0.06
Dibutylphenylthioborane	76.46	76.82	-0.36	-0.47
Dichloro 4-chlorobutoxyborine	40.73	40.65	0.08	0.20
Dichloro butoxyborine	36.03	35.85	0.18	0.50
Dichloro isobutoxyborine	36.55	35.81	0.74	2.02
Dichloro neopentoxyborine	40.51	40.46	0.05	0.12
Dichloro octoxyborine	53.85	54.37	-0.52	-0.97
Dichloro propoxyborine	30.62	31.22	-0.60	-1.96
Diisoamylbutylthioborane	79.99	79.90	0.09	0.11
Diisobutylboronic anhydride	87.73	87.03	0.70	0.80
Diisobutylbutylthioborane	71.06	70.64	0.42	0.59
Diisopentylboronic anhydride	105.56	105.55	0.01	0.01
Diisopropylboronic anhydride	68.78	68.75	0.03	0.04
Dioctyl butoxyborine	100.02	100.79	-0.77	-0.77
Dipropylbutylthioborane	61.51	61.46	0.05	0.08
Dipropylethylthioborane	52.48	52.20	0.28	0.53
Dipropylisobutylaminoborane	55.99	56.09	-0.10	-0.18
Dipropylphenylaminoborane	63.31	63.31	0.00	0.00
Dipropylphenylthioborane	67.67	67.56	0.11	0.16
Ethyl phenyl butoxyborine	61.09	61.05	0.04	0.07
Ethylphenylboronic acid	42.13	41.55	0.58	1.38
Ethylphenylboronic anhydride	82.57	81.79	0.78	0.94
Ethylthio dioctyl borane	98.03	98.50	-0.47	-0.48
Ethylthiodiethylborane	42.82	42.94	-0.12	-0.28
Hexyldichloroborane	44.07	44.03	0.04	0.09
Isobutyl cyclohexylchloroboronate	56.96	56.76	0.20	0.35
o-Tolylamino(diethylamino)borane	63.48	63.31	0.17	0.27
Pentyldichloroborane	39.49	39.40	0.09	0.23
Phenyl 2-tolyl propoxyborine	77.12	77.05	0.07	0.09
Phenyl di(sec-butoxy)borine	71.45	71.64	-0.19	-0.27
Phenyl di(sec-octoxy)borine	108.55	108.68	-0.13	-0.12
Phenyl dibutoxyborine	71.32	71.62	-0.30	-0.42
Phenyl diethoxyborine	52.87	53.10	-0.23	-0.44
Phenyl diisobutoxyborine	71.44	71.54	-0.10	-0.14

Phenyl dimethoxyborine	43.45	43.78	-0.33	-0.76
Phenyl dipropoxyborine	62.40	62.36	0.04	0.06
Phenylamino(diethylamino)borane	58.85	58.50	0.35	0.59
Phenylboron dichloride	41.64	41.33	0.31	0.74
Phenylpropylboronic acid	46.40	46.18	0.22	0.47
Phenylpropylboronic anhydride	90.30	91.05	-0.75	-0.83
Tri(1,2,2-trimethylpropoxy)borine	93.61	94.28	-0.67	-0.72
Tri(1,3-dichloro-2-propoxy)borine	81.12	81.47	-0.35	-0.43
Tri(1-chloroethoxy)borine	52.99	53.51	-0.52	-0.98
Tri(1-ethoxycarbonylethoxy)borine	85.93	85.70	0.23	0.27
Tri(1-methoxyethoxy)borine	57.42	57.14	0.28	0.49
Tri(2-ethoxycarbonylethoxy)borine	84.97	85.67	-0.70	-0.82
Tri(2-pentoxy)borine	80.11	80.45	-0.34	-0.42
Tri(butylthio)borane	87.47	87.36	0.11	0.13
Tri(ethoxycarbonylmethoxy)borine	71.14	71.78	-0.64	-0.90
Tri(propylthio)borane	73.47	73.47	0.00	0.00
Tri(t-butoxy)borine	66.77	66.38	0.39	0.58
Tributyl borate	66.65	66.53	0.12	0.18
Tridecyl borate	149.41	149.87	-0.46	-0.31
Triethyl borate	38.69	38.75	-0.06	-0.16
Triethylborane	33.72	34.51	-0.79	-2.34
Triheptyl borate	109.18	108.20	0.98	0.90
Triisobutylborane	62.31	62.17	0.14	0.22
Triisopentoxyborine	80.14	80.30	-0.16	-0.20
Triisopentylborane	76.54	76.06	0.48	0.63
Triisopropyl borate	52.52	52.67	-0.15	-0.29
Trimethoxyborine	24.86	24.77	0.09	0.36
Trioctyl borate	122.30	122.09	0.21	0.17
Tripentoxyborine	80.42	80.42	0.00	0.00
Tripropyl borate	52.55	52.64	-0.09	-0.17
Tripropylborane	48.54	48.40	0.14	0.29
Tris(ethylthio)borane	59.41	59.58	-0.17	-0.29

4.2. Polarizability

The calculation of the molecular polarizabilities has been carried out indirectly via the calculated refractivities applying the inverse Lorentz-Lorenz relation. In order to include the relatively limited number of experimentally determined polarizability data in the atom-group parameters and any further calculations, they have been translated into the corresponding refractivity values and henceforth treated just like the remaining experimental refractivities. Conversely, all the experimental refractivity values have been analogously converted into "experimental" polarizabilities. The complete set of true and indirectly determined experimental

polarizability values is compared in Fig. 4 with the indirectly calculated polarizability values, mirroring the excellent correlation of Fig. 2, which at first sight is not surprising as both value sets are multiplied with the same factor. However, we should not forget that the truly experimentally determined polarizability values have been evaluated by various methods that differ from those for the experimental determination of the refractivity. In fact, as the histogram in Fig. 5 reveals, it turned out that 23 compounds should be viewed as outliers because their experimental refractivity values deviated by more the three times the standard deviation σ of $0.15 \text{ \AA}^3$ from calculations. They are collected in a separate list, available in the Supplementary Materials, together with the complete set of compounds with experimental and calculated polarizabilities.

In a paper of Tariq et al. [276], the applicability of the Lorentz-Lorenz relation has been questioned for ILs because it is based on the assumption of the compounds being "isotropic fluids composed of spherical and non-interacting particles" which is not given with this class of salts, since at least one of its ions is non-spherical, and they are clearly non-isotropic fluids as they consist of polar centers surrounded by non-polar moieties. These considerations are certainly justified with respect to the relationship between refractivity and polarizability of ILs. In the following section, however, we will demonstrate that the non-spherical character of the ILs is no obstacle for a reasonable correlation between molecular volume and refractivity.

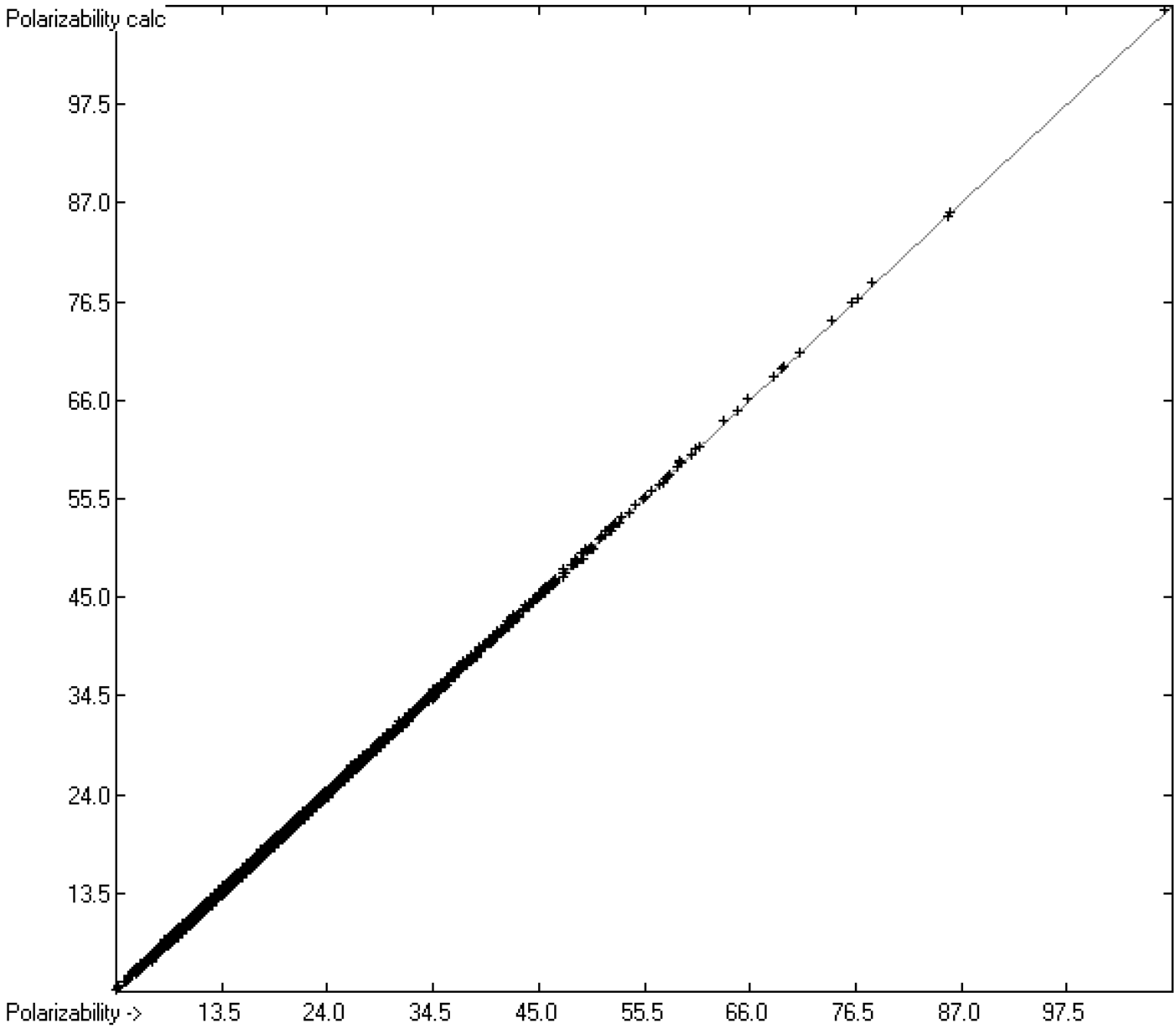


Figure 4. Correlation diagram of the polarizability data (in Å³).
(N =5763, R² = 0.9997, regression line: intercept =0.0115; slope =0.9995, MAPD=0.72%).

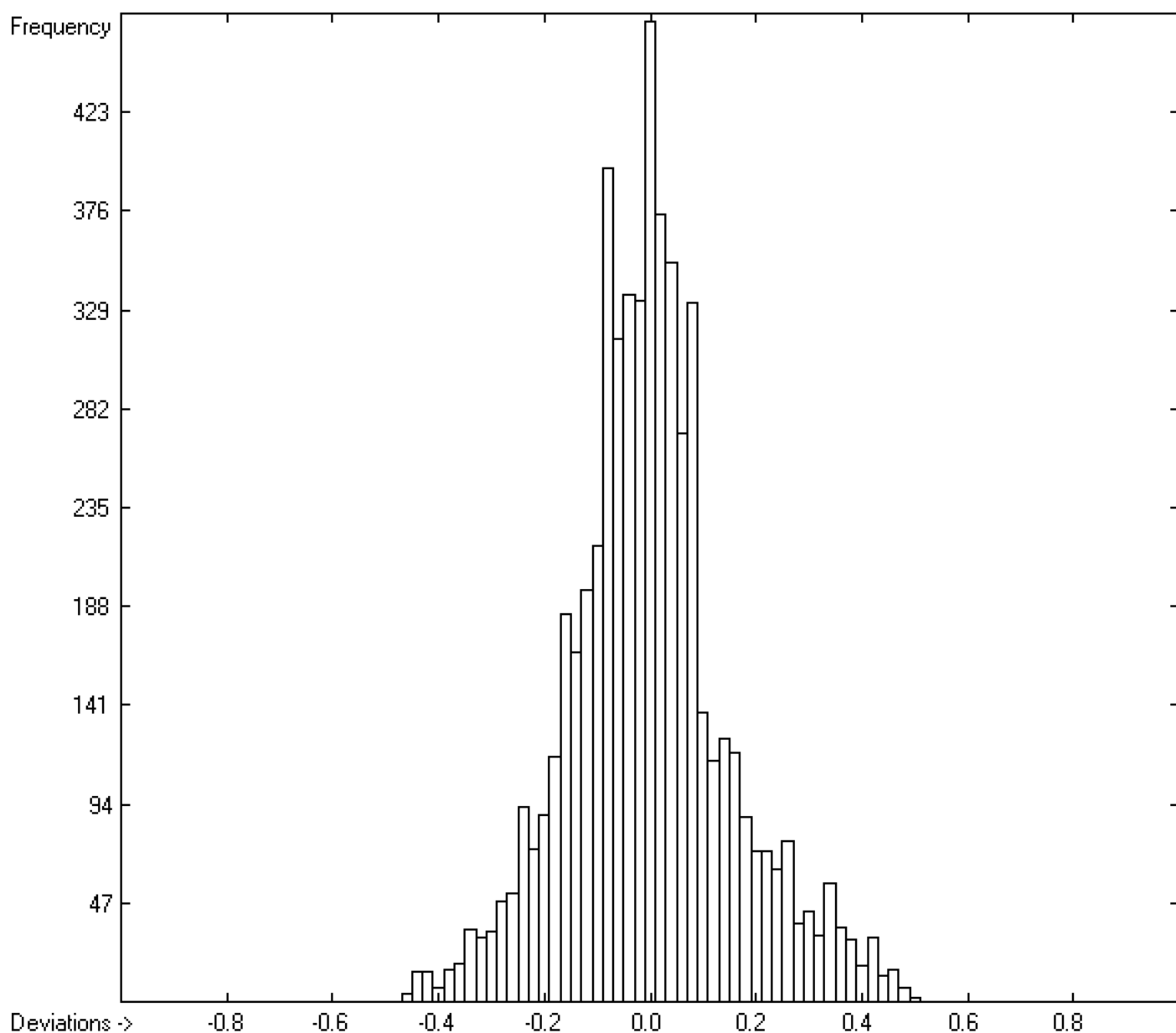


Figure 5. Histogram of the polarizability data ($\sigma = 0.15 \text{ \AA}^3$; exp. values range from 3.23 to 107.53 $\text{\AA}^3$).

4.3. Refractivity/Polarizability and Molecular Volume

A paper of Brinck et al. [6] discussed the relationship between the polarizability of a molecule and its volume, arguing that physically "the polarizability α of a conducting sphere of radius R is equal to R^3 ", its relation expressed by the equation $\alpha = 3V/4\pi$, where V is the volume. This relation is true on condition that the electrostatic potential is uniform within this sphere, which is certainly not the case in a molecule. An approximate equation, known as the Clausius-Mosotti equation, proposes for nonpolar molecules the polarizability as being directly proportional to their volume and a function of their dielectric constant. Several approaches for the calculation of the molecular volumes have been chosen in order to assess their applicability for polarizability predictions. Gough [408], Laidig and Bader [409] and Brinck et al. [6] used various Hartree-Fock self-consistent field methods to compute the volumes of a limited number of small molecules and achieved good linearity with their polarizability, depending on the size of the contour of the electronic density defining the molecule's surface. In an earlier paper [7], we presented a fast numerical method for the calculation of the "true" molecular volume of molecules of any size and type, including ILs, based on the

atoms' Van-der-Waals radii. Since these "true" (elsewhere also called "hardcore") volumes are automatically generated on entering a new compound to the database, it was obvious to examine their potential linearity with their experimental polarizability or refractivity as far as available. In Fig. 6 the correlation between the "true" molecular volume and the experimental refractivity of 6069 molecules is shown, revealing an excellent correlation coefficient R^2 of 0.9645 and a MAPD of 7.53%. Fig. 7 presents the same correlation diagram, but restricted to the class of ILs, indicating that the path of prediction of their refractivity R via their molecular volume V as calculated in [7] and applying the simple linear equation $R = \text{intercept} + (V \times \text{slope})$ provides a reliable refractivity value with a MAPD of little more than 5% within the ILs class over a large range of molecular volumes, if the atom-group additivity method does not allow a calculation due to the limitations mentioned earlier. The complete list of molecules with their "true" molecular volume and experimental and volume-derived refractivity is available in the Supplementary Materials.

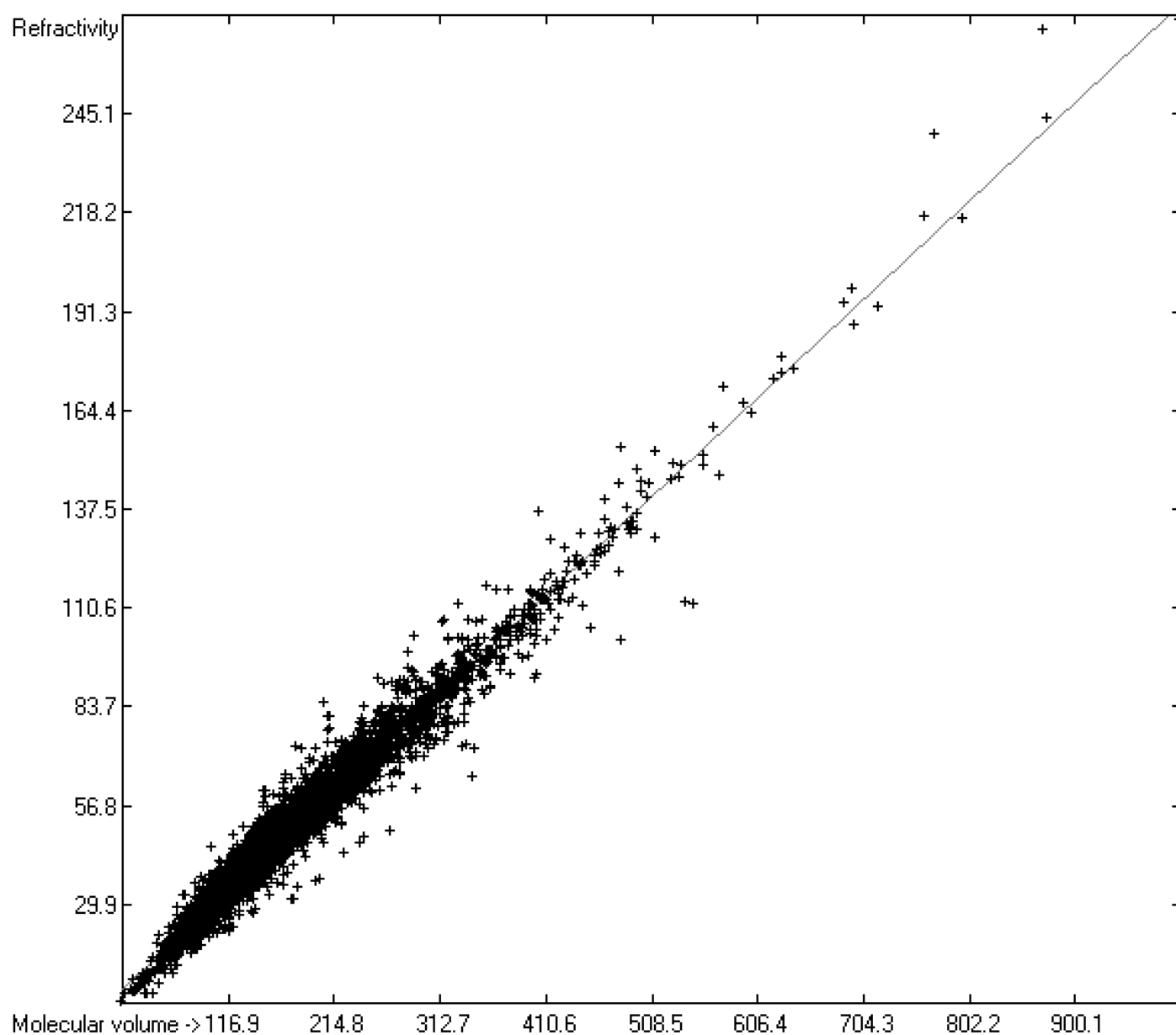


Figure 6. Correlation diagram of "true" molecular volume [7] vs. experimental refractivity. (N =6069, R^2 =0.9645, regression line: intercept = 1.4354; slope =0.2743, MAPD=7.53%).

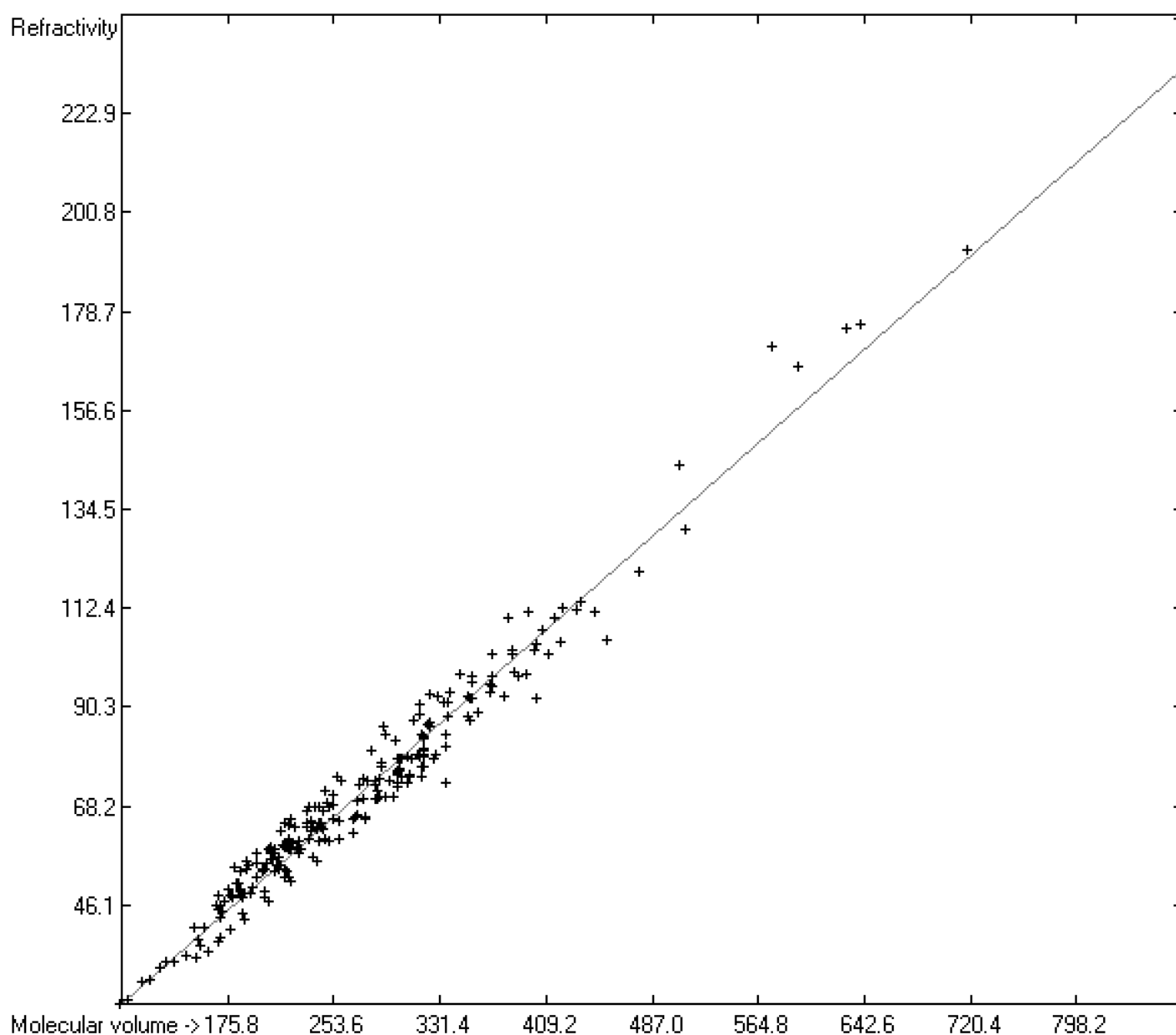


Figure 7. Correlation diagram of "true" molecular volume [7] vs. experimental refractivity of ILs. (N =247, $R^2 = 0.9700$, regression line: intercept = -2.4557; slope = 0.2686, MAPD=5.35%).

5. Conclusions

In several earlier papers [1, 7, 8, 403-407], the present atom-groups additivity algorithm, outlined in [1], has proven its formidable versatility for the reliable prediction of up to 17 physical, thermodynamic, solubility-, optics-, charge-, and environment-related descriptors. In the present work, which is part of an ongoing project, the results of the present refractivity/polarizability calculations again demonstrate its as-yet unsurpassed accuracy and easy expandability. The nearly 6'000 molecules providing their experimental refractivity or polarizability values, either directly or via their refractive index and density, enabled the calculation of a large set of atom-group parameters allowing the refractivity/polarizability of nearly 80% of the compounds listed in a database of presently approaching 36'000 of nearly any molecular structure, size and application. The big advantage of the present method is the basic possibility to calculate the refractivity simply by means of paper and pencil applying the parameters set listed in Table 2. In addition, we have shown that optionally refractivity/polarizability calculations are possible via the molecular-volume route - although with lower accuracy - in cases where the group-additivity method is disabled.

The mentioned project's software is called ChemBrain IXL, available from Neuronix Software (www.neuronix.ch, Rudolf Naef, Lupsingen, Switzerland).

Supplementary Materials

The list of compounds used in the present work, their experimental data and 3D structures are available online as standard SDF files, accessible for external chemistry software, under the name of "S01. Compounds List for Refractivity-Parameters Calculations.sdf". The list of the compounds used in the correlation diagrams and histograms containing their names and their experimental and calculated values are available under the corresponding names of "S02. Experimental vs. Calculated Refractivities.doc", "S03. Experimental vs. Calculated Polarizabilities.doc" and "S04. Molecular Volume vs. Refractivity Data Table.doc". Separate analogous lists are available for ionic liquids under the name of "S05. Experimental vs. Calculated Refractivities of Ionic Liquids.doc", for silicon compounds under the name of " S06. Experimental vs. Calculated Refractivities of Silicon Compounds.doc", and for boron compounds under the name of " S07. Experimental vs. Calculated Refractivities of Boron Compounds.doc". In addition, two lists containing the outliers in the calculations of the refractivity and polarizability of molecules are available under the names of "S08. Refractivity Outliers.doc" and "S09. Polarizability outliers.doc". Finally, the figures are available as .tif files and the tables as .doc files under the names given in the text.

Author Contributions

R. Naef developed project ChemBrain and its software upon which this paper is based, and also fed the database, calculated and analysed the results and wrote the paper. W. E. Acree suggested the extension of ChemBrain's tool and contributed experimental data and the great majority of the literature references. Beyond this, R. Naef is indebted to W. E. Acree for the many valuable discussions.

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Conflicts of Interest

The authors declare no conflict of interest.

Sample Availability: Samples of the compounds are not available from the authors.

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