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Second-Order Group Contribution Method for the Determination of the Dipole Moment

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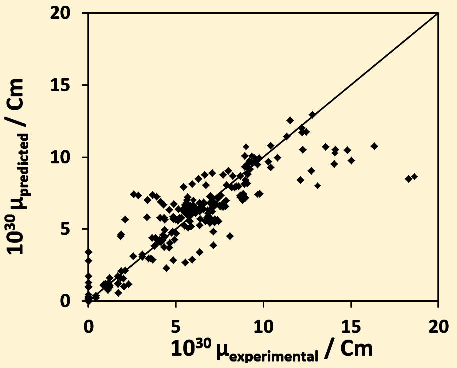
Supporting Information

ABSTRACT: An estimation method for the dipole moment is proposed in this work. Polarity is caused by the effect of different neighboring groups in a molecule. A second-order group contribution approach has been chosen due to its ability to account for this effect. It could be shown that the use of second-order groups can cause a significant increase in prediction quality compared to the conventional first-order approach. The prediction quality of the proposed method is good, even for higher values of the dipole moment. Those higher than about 3.5 D are however underestimated. The model also enables the prediction of the small but finite dipole moments of hydrocarbons. Adequate estimations are not limited to compounds from the training set, but also compounds from a test set show good prediction results. Hence, it can be concluded that this method is able to give quick and reliable predictions for not yet measured dipole moments.



1. INTRODUCTION

The dipole moment is a substance property that is used in many fields of chemical engineering, e.g., the determination of second virial coefficients by the Hayden O'Connell model[1] or the prediction of solubility.[2] The dipole moment can be experimentally determined by measuring the permittivity[3] or by using the Stark-effect.[4] Nevertheless, experimental data for the dipole moment are often not available. Hence, it is desired to estimate them based on structural information of the respective molecule or on other experimental data that are more commonly available in literature.

Quantum mechanics and molecular mechanics offer an opportunity to predict dipole moments directly from the conformational analysis. If an appropriate method and parametrization are chosen, good predictions can be achieved using these approaches.[5] The error (root-mean-square deviation) given by Moreno-Mañas[6] for β-diketones varies between (0.25 and 1.19) D depending on the method applied. Due to parametrization, some of the quantum-chemical methods are limited to specific substance classes (e.g., CHIH-DFT[7] is applicable to heterocyclic compounds only). So to make the adequate predictions, one needs an extended specific knowledge, the corresponding software, and time.

An easier and faster way for determining substance properties are group contribution methods. Fishtine[8] already presented an early form of a group contribution approach concerning the dipole moment in 1963. This method is limited to aromatic compounds with the errors ranging between (2 and 30) %.[9] In 2005, Sheldon et al.[2] presented a first-order group contribution method that predicts dipole moments for most substance classes from group contributions and the molar volume of the respective compound. This model is able to give good results for medium values of the dipole moment. For slightly polar compounds the dipole moment is significantly overestimated. Dipole moments higher than 2 D are usually underestimated.

The model of Sheldon et al. is based on first-order group contributions. This means that groups are viewed as being isolated and the effects of their next neighbors are not taken into account. The polarity of a molecule is caused by the separation of electric charges due to different electronegativity of neighboring and nearby atoms. Hence, in order to achieve good modeling results, determination of the dipole moment should consider not only the functional groups that built the compound but also the effect of the next neighbors (2nd order method). A second-order group contribution model for substance properties has first been developed by Benson and Russ for caloric properties.[10] In such a model, the first-order group CH_3-, for example, can be differentiated in different second-order groups such as a CH_3-group next to a sp^3-carbon atom $CH_3-(C)$, next to a double bounded carbon atom $CH_3-(C{=})$, next to an aromatic carbon atom $CH_3-(aC)$, next to a carbonyl group $CH_3-(CO)$ or next to an oxygen atom $CH_3-(O)$ and so on. The number of possible second-order groups can be even higher for, e.g., a CH_2 group, since two neighboring groups are connected to the CH_2 group. By differentiating the groups in this way, a second-order group contribution method is able to comprise the effects of neighboring atoms of different electronegativity, which is the major reason for the formation of permanent dipoles. Thus, in this work, the approach of Sheldon et al.[2] has been extended to a second-order method.

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2. DETERMINATION OF THE PARAMETERS

2.1. Experimental Database. Experimental data for different compounds were derived from the DIPPR database,[11] Yaws,[12] and Poling et al.[13] The substances were divided into two groups: the training set for the adjustment of the parameters consisted of 90 % of the substances. A total of 10 % of the substances were kept for a test set and did not become part of the training set. The test set was later used to evaluate the predictive quality of the model and the parameters. The selection of the test set was based on the assumption that each major class of substances (ether, ester, aromatics, nitrogen-, halogen-containing-compounds, and so on) should be part of the test set.

The training set consisted of 233 compounds, the test set of 26 compounds. The number of groups of the compounds from the training set ranged from 2 to 18 with an average group number of 5.8. A total of 54 compounds consisted of carbon- and hydrogen atoms only. A total of 101 compounds contained carbon-, hydrogen-, and oxygen-atoms. A total of 44 compounds contained halogens and 34 contained nitrogen as well. The dipole moments ranged from (0 to 5.486) D. The relative frequency P of the different dipole moments in the training set and the test set can be seen from Figure 1.

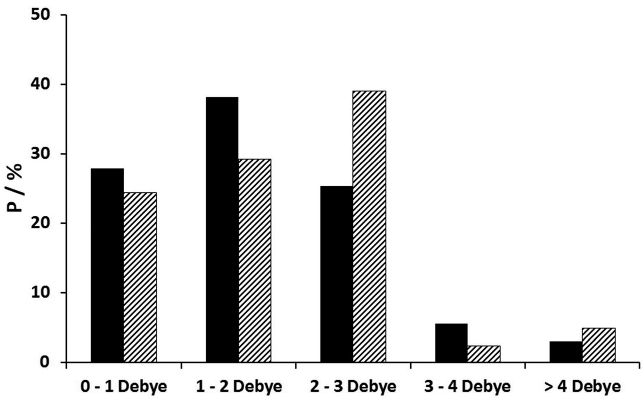

Figure 1. Relative frequency P of different dipole moments in the training set (black bars) and in the test set (ruled bars).

The substances were assigned into second-order groups. If a group was present in one compound only, it was not considered, since no reliable parameter fitting could be guaranteed. Nevertheless, the number of compounds containing a specific group strongly varied. The $CH_3-(C)$ group, for example, was present in 114 compounds, whereas the $CH_3-(aC)$ group was present in 16 compounds only.

In addition to the conventional second-order groups, corrections for special structures were added. These corrections were treated like the other groups but contribute to effects like the polarity caused by substitution of an aromatic ring in ortho-position.

2.2. Parameter Fitting and Error Analysis. The group contributions as well as the other model parameters have been fitted to the experimental data by the least-squares method using an Levenberg–Marquardt algorithm.[14] This approach supports the parameter fitting especially with respect for high dipole moment values. The sum of the squares of the errors is minimized by varying the group contributions represented by the parameter vector $\vec{B}$.

$$\min_{\vec{c}} \sum_{j=1}^{n} (\mu(\vec{g}_j, \vec{B}) - \mu_{j,\text{experimental}})^2 \tag{1}$$

where $\mu(\vec{g}_j,\vec{B})$ is the predicted dipole moment of compound j and $\mu_{j,\text{experimental}}$ is its experimental value. The vector $\vec{g}_j$ represents the group assignment to compound j. The minimization was first done for the group contributions using fixed parameters in the correlation function (eq 5). Afterward, the correlation parameters in the estimation functions were fitted analogously. This procedure was repeated until convergence was reached. Additional parameters that account for effects of substance class and size have been fitted afterward using the same algorithm.

The quality of the prediction has been evaluated by looking at three different measures of errors. The average absolute error (AAE) was calculated as

$$\text{AAE} = \frac{\sum_{i=1}^{n} |\mu_{i,\text{experimental}} - \mu_{i,\text{predicted}}|}{n} \tag{2}$$

where n is the number of compounds analyzed and $\mu_{\text{predicted}}$ is the value estimated using the proposed model. The AAE weights all errors equally, so that the errors on small dipole moments are not considered appropriately. To account for this effect, the errors were also evaluated relative to the absolute value of the dipole moment by using the average absolute percentage error (AAPE)

$$\text{AAPE} = \frac{100\%}{n} \sum_{i=1}^{n} \frac{|\mu_{i,\text{experimental}} - \mu_{i,\text{predicted}}|}{\mu_{i,\text{experimental}}} \tag{3}$$

For the calculation of the AAPE, only compounds with an experimental value of the dipole moment unequal to zero are taken into account to avoid division by zero.

The root-mean-square deviation (rmsd) as a third measure of error was calculated as

$$\text{RMSD} = \sqrt{\frac{\sum_{i=1}^{n} (\mu_{i,\text{experimental}} - \mu_{i,\text{predicted}})^2}{n}} \tag{4}$$

The rmsd weights huge errors more than small ones and therefore is a measure for the probability of huge discrepancies.

3. RESULTS

Group contribution methods are usually suited well for estimating energetic properties, but give poor results for nonenergetic properties. Therefore, it is reasonable to describe the dipole moment as a function of energetic properties that are calculated from group contributions and nonenergetic properties that are input parameters and not estimated within the model. The dipole moment can be correlated to the cohesive energy density δ_P and the molar volume v. Therefore, the correlation function should be a product of these quantities to the power of appropriate correlation parameters (eq 5) as suggested by Koenhen and Smolders:[15]

$$\mu = a\delta_P^b v^c \tag{5}$$

The molar volume is a substance property for which experimental data often are available, even if no dipole moment is found. If no experimental values for the molar volume are

Table 1. List of Group Contributions B_i

group	B_i	group	B_i	group	B_i
	$J\cdot cm^{-3}$		$J\cdot cm^{-3}$		$J\cdot cm^{-3}$
CH_3 groups		unsaturated groups		carbonyl groups	
CH_3—(C)	0.0	$=CH_2$	26.8	CHO—(C)	453898.3
CH_3—(C=)	5388.0	=CH—(C)	−8697.7	CHO—(C=)	1027492.8
CH_3—(aC)	327778.7	=CH—(C=)	−3336.4	CHO—(O)	237963.6
CH_3—(O)	−13820.7	=CH—(O)	18357.7	CO—(2C)	833743.0
CH_3—(CO)	24657.5	=CH—(CO)	129809.8	CO—(C,O)	198667.5
CH_3—(N)	−1065.8	=CH—(X)	−52005.2	CO—(=C,O)	326445.4
CH_2 groups		=C—(C,CO)	−8170.3	CO—(aC,O)	677211.4
CH_2—(2C)	−50.7	=C—(2C)	−7181.2	CO—(2O)	385693.2
CH_2—(C,C=)	1039.6	=C—(2X)	31151.7	COOH—(C)	100538.8
CH_2—(C,aC)	327779.4	aromatic groups		COOH—(=C)	125403.9
CH_2—(C,O)	5850.7	aCH	−3585.6	COOH—(aC)	311033.6
CH_2—(C,CO)	77340.0	aC—(C)	−329254.1	N groups	
CH_2—(C,N)	−21105.9	aC—(aC)	8965.1	NH_2—(C)	78202.5
CH_2—(C,X)	60877.3	aC—(O)	51335.4	NH_2—(aC)	−39199.4
CH_2—(CO,X)	4329.2	aC—(CO)	−97362.1	NH—(2C)	−112258.7
CH groups		aC—(N)	215336.2	NO_2—(C)	1722454.9
CH—(3C)	23.4	O groups		NO_2—(aC)	1137898.8
CH—(2C,O)	−4447.7	OH—(C)	266210.1	corrections	
CH—(2C,CO)	−26921.9	OH—(aC)	134566.6	3-membered ring	152.2
CH—(2C,N)	9375.9	O—(2C)	64572.5	5-membered ring	179.4
CH—(2C,X)	65030.4	O—(C,=C)	44024.9	6-membered ring	−3990.5
CH—(C,2X)	−103426.2	O—(C,CO)	18657.9	heterocyclic	390453.5
CH—(C,O,CO)	338105.0	halogen groups		cis	7473.9
C groups		F—(C)	166965.9	trans	6619.0
C—(4C)	50.7	F—(=C)	80312.6	ortho	24890.2
C—(3C,O)	−42084.6	Cl—(C)	127016.6	meta	18311.1
C—(C,2X,Y)	−757036.8	Cl—(C=)	−43397.4	para	17291.8
C—(C,3X)	−500897.4	Br—(C)	100304.2		

available, other prediction methods could be used (e.g., ref 16). However, using these data for the dipole moment prediction should be done with care.

The value of δ_P is calculated in this model by eq 6

$$\delta_P = \sum_i n_i B_i \tag{6}$$

where n_i is the number of group i in the respective molecule and B_i is the contribution of the group to δ_P. So, e.g., for m-cresole, δ_P can be calculated as

$$\delta_{P,m-\mathrm{cresole}} = 4B_{\mathrm{aCH}} + 1B_{\mathrm{aC-(C)}} + 1B_{\mathrm{CH3-(aC)}} + 1B_{\mathrm{aC-(O)}} + 1B_{\mathrm{OH-(aC)}} + 1B_{\mathrm{meta}} \tag{7}$$

The parameters a, b, and c in eq 5 have been determined as $a = 0.076\ \mathrm{D\ cm^{1.326}\ mol^{-0.133}\ J^{-0.309}}$, $b = 0.309$, and $c = -0.133$ (1D ≈ 3.33564×10^{-30} C·m). Values for the group contributions B_i can be taken from Table 1. In Table 1, "aC" denotes an aromatic carbon atom, X denotes a halogen, X and Y denote a substitution of one group by two different halogens. For benzene-rings, no "6-membered ring" correction is used.

For the example of m-cresole, δ_P gives

$$\delta_{P,m-\mathrm{cresole}} = 4(-3585.6) + 1(-329254.1) + 1(327778.7) + 1(51335.4) + 1(134566.6) + 1(18311.1)$$

$$\delta_{P,m-\mathrm{cresole}} = 188395.3\ \frac{\mathrm{J}}{\mathrm{cm^3}} \tag{8}$$

For a molar volume of 104.4 $\mathrm{cm^3/mol}$ of m-cresole, the dipole moment can be calculated as

$$\mu_{m-\mathrm{cresole}} = 0.076\ \frac{\mathrm{D\ cm^{1.326}}}{\mathrm{mol^{0.133}\cdot J^{0.309}}}\left(188395.3\frac{\mathrm{J}}{\mathrm{cm^3}}\right)^{0.309}\left(104.4\ \frac{\mathrm{cm^3}}{\mathrm{mol}}\right)^{-0.133}$$

$$\mu_{m-\mathrm{cresole}} = 1.75\ \mathrm{D} \tag{9}$$

The experimental value is 1.59 D,[11] which means a deviation of 9.9 %.

Different additional parameters and group contributions with respect to effects of substance classes and molecule size have also been evaluated. Some additional parameters (e.g., a substance class correction to parameter c for alkanes and esters) would allow for better reproduction of the dipole moments from the training set. Nevertheless, the implementation of additional parameters or further group contributions did not yield a significant increase in accuracy of prediction within the test set. Hence, it was decided not to use further parameters for the model.

To simplify the method, the effect of the molar volume could be principally ignored in eq 5. As a consequence, it was tested if prediction is possible with the factor containing the molar volume being set to one. Parameter fitting was successful and the experimental data could be reproduced. However, quality of prediction significantly decreases as it could also be expected theoretically. Therefore, it was decided not to ignore the influence of the molar volume.

Sheldon et al.[2] set the dipole moment to zero for all compounds that contain C and H atoms only. For *n*-alkanes, this is a reasonable statement. However, an error occurs for alkenes, branched alkanes, and alkylbenzenes with small but finite dipole moments. Therefore, in our model, we set to zero the dipole moments only of *n*-alkanes and *n*-alkanes with all hydrogen atoms substituted by the same halogen atom but not for other hydrocarbons. Additionally, planar molecules that can be brought into at least two indistinguishable forms by rotation in the plane (e.g., benzene, perchlorobenzene, *trans*-dichloroethylene, compounds consisting of an aromatic ring with the same substituents twice in para position or three times in 1,3,5 position, etc.) and nonpolar molecules that exhibit indistinguishabilities by rotation around at least two axes (e.g., 2,2-dimethylpropane but not chloromethane since it only shows indistinguishable forms by rotation around one axis) are forced to have zero dipole moments as well.

4. DISCUSSION

A plot that shows predicted dipole moments versus experimental data can be seen in Figure 2. The parity plot for the compounds from the training set is given in Figure 2a and for those from the test set in Figure 2b. As seen, the method is able to reproduce the values not only for the compounds from the training set but also to predict values for substances from the test set.

Unlike the model of Sheldon et al.,[2] our method is able to give good prediction results not only for lower values of the dipole moment, but also for dipole moments higher than 2 D. For dipole moments higher than about 3.5 D, our model seems to underestimate the dipole moment. Calculations of small, but finite dipole moments (<1 D) could be enabled since values for slightly polar hydrocarbons are not generally set to zero.

Predictions for hydrocarbons exhibit only slight deviations from the experimental data. For compounds containing other elements, the prediction is good in most cases. However, some data points show a greater deviation from the diagonal. Within the group of the oxygen containing substances, the highest deviance is exhibited by some organic acids and compounds containing more than one hydroxyl group. For some multi-halogenated compounds a similar effect was observed. In this case, prediction quality is generally high for compounds that contained halogen atoms attached only to the same carbon atom. For compounds containing two or more halogen atoms placed at different C-atoms, the deviation from the diagonal increases. Prediction for nitrogen-containing substances is usually good. The outliers within this class can be assigned to aromatic compounds containing NO_2- and another highly electronegative group at the same time (e.g., nitroaniline). Summing this up, it can be stated that the method can give reliable prediction results. Nevertheless, predictions for substances carrying two or more substituents with high electronegativity should be handled with care.

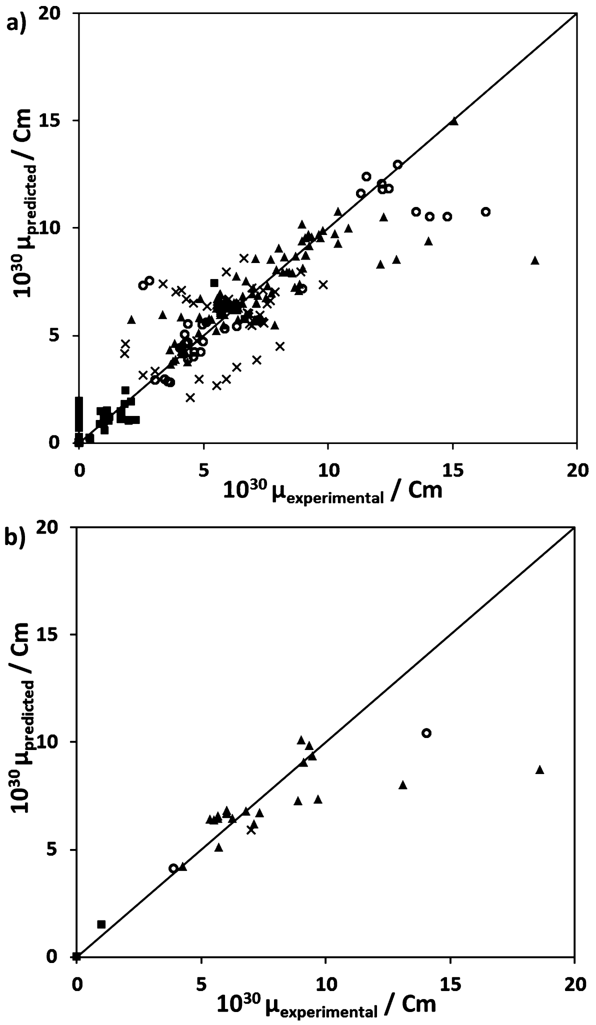

Figure 2. Predicted dipole moment $\mu_{\text{predicted}}$ vs experimental dipole moments $\mu_{\text{experimental}}$ for compounds from the training set (a) and the test set (b) (squares: hydrocarbons, triangles: oxygen-containing compounds, crosses: halogen-containing compounds, circles: nitrogen-containing compounds).

The errors are independent of the size of the molecule within the range of the compounds tested. Therefore, it can be concluded that the estimation method is valid for a broad range of molecules independent of their size.

Results for three C_4-hydrocarbons are depicted in Figure 3 along with the results of quantum-chemical calculations as presented by Tasi et al.[17] The prediction quality is high in all cases for the proposed method as well as for the quantum-chemical approach. The first gives slightly better predictions for 2-methyl propene, while the later one is marginally better for methyl propane. On *cis*-2-butene the absolute error is similar for both models. So in terms of accuracy, none of the approaches is clearly superior. The advantage of the group contribution method lies in its ease of use and the low requirements concerning time and computational capacities. Note that the model suggested by Sheldon et al.[2] sets the dipole moments of all three substances to zero.

To directly illustrate the benefit of a second-order group contribution approach for the dipole moment over a first-order modeling,[2] results of calculations for some compounds are

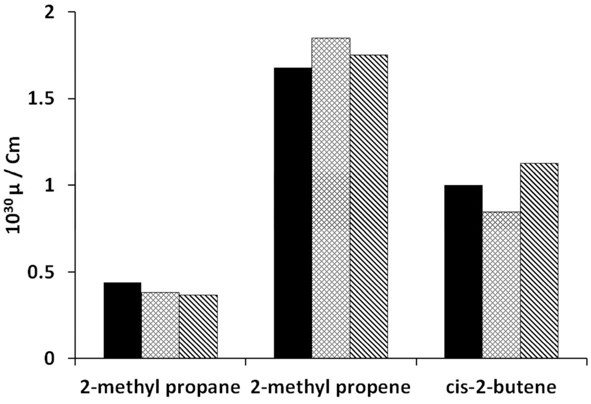

Figure 3. Dipole moments (μ) calculated by a quantum-chemical approach (checkered bars) and second-order group contributions (ruled bars) compared to experimental values (black bars).

shown exemplarily in Figure 4. The considered substances consist of two methyl groups attached to another functional group (CH_2, O, C=O, NH, and C=). Since both methods automatically set the dipole moment of propane to zero, they both give the same correct value for this compound. For 2-methyl propene, the zeroing made in Sheldon's approach gives a clear misestimation, while the proposed method can well reproduce the low but finite value (experimental: 0.5 D; calculated 0.53 D). For propanone and dimethyl amine, the first-order model can give a fair estimation [(2.3 and 1.3) D, respectively)] of the experimental values [(2.88 and 1.03) D, respectively]. Taking into account the effect of the neighboring groups by applying the proposed second-order method, an increase in prediction quality can be reached [(2.94 and 0.9) D, respectively]. The absolute error therefore is decreased by (89 and 56) %, respectively. In the case of dimethyl ether, both methods give good predictions (experimental: 1.3 D; first-order: 1.26 D; second-order: 1.13 D). Although the prediction by the first-order approach is slightly better than the one using the proposed method, generally the latter is able to give a better prediction (see also Table 2).

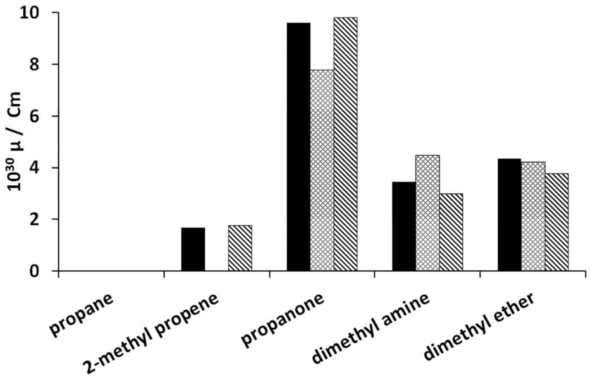

Figure 4. Dipole moments (μ) of some compounds containing two methyl groups attached to another functional group (black bars: experimental data, checkered bars: values calculated from the first-order group contributions,[2] ruled bars: values calculated from the second-order group contributions).

To allow for a comparison based on a larger database an overview of the errors is given in Table 2. The training set of Sheldon et al.[2] is unknown and no error analysis for a test set is given. To allow for a comparison on the same substances, the errors for these models are given for the compounds of our test set. The values for the errors given in the respective publication[2] are calculated for different compounds and thus in some cases are slightly different but within the same magnitude.

Table 2. Errors for the Proposed Method in Comparison to the Method of Sheldon et al.[2]

	10^{30}·rmsd	AAPE	10^{30}·AAE
	C·m	%	C·m
proposed method training set (233 compounds)	1.57	18	0.97
proposed method test set (26 compounds)	2.47	15	1.37
Sheldon et al.[2] applied on our test set (26 compounds)	3.3	26	1.90

It can be seen that the errors for the test set are in general higher than those for the training set. Only the relative error AAPE exhibits a slightly lower value for the test set. The method of Sheldon et al.[2] gives higher values for all error measures. For the rmsd and the AAE, the error of the first-order approach is (30 to 40) % higher than for the proposed second-order approach. Its AAPE exceeds the error of the new method by even more than 60 %. These show that the developed method gives better predictions for the whole range of dipole moments and for the low values especially (alkenes, alkylbenzenes, etc.).

So the progression from a description of the substances using first-order groups to the use of second-order groups can improve the accuracy of the prediction.

5. CONCLUSION

The group contribution method for the prediction of the dipole moment proposed by Sheldon et al.[2] has successfully been extended to a second-order group contribution model. Group contributions for compounds containing carbon, hydrogen, oxygen, nitrogen, and halogens have been determined so far. Unlike first-order groups, the second-order groups can account for the effects of neighboring atoms, which are the main reasons for polarity. Structural corrections for rings and substitution position turned out to be able to significantly improve the determination. Introduction of further corrections for substance class and molecule size did not give additional improvements in the prediction quality.

The prediction quality could be improved for lower as well as for higher dipole moments. Estimation was possible not only for compounds from the training set, but prediction results were also good for compounds from the test set. Hence, it can be concluded that the method is able to give quick predictions for dipole moments not yet measured.

■ ASSOCIATED CONTENT

Supporting Information

Table containing experimental data used and results of the predictions. This material is available free of charge via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

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