



# Limiting Diffusion Coefficients for Ions and Nonelectrolytes in Solvents Water, Methanol, Ethanol, Propan-1-ol, Butan-1-ol, Octan-1-ol, Propanone and Acetonitrile at 298 K, Analyzed Using Abraham Descriptors

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## Abstract

We have used literature data on the conductivity of single ions to obtain limiting diffusion coefficients ( $D^0$ ) of ions in water, alcohols, propanone and acetonitrile. We then used literature data on limiting diffusion coefficients of nonelectrolytes in order to set up linear free energy relationships that combine data for ions and nonelectrolytes, as  $\log_{10}(D^0)$  in the same equation, all values being at 298 K. These equations are for solvents water ( $N=377$ ,  $SD=0.0474$ ), methanol ( $N=96$ ,  $SD=0.0332$ ), ethanol ( $N=96$ ,  $SD=0.0666$ ), propan-1-ol ( $N=71$ ,  $SD=0.0487$ ), butan-1-ol ( $N=53$ ,  $SD=0.0600$ ), octan-1-ol ( $N=61$ ,  $SD=0.0684$ ), propanone ( $N=86$ ,  $SD=0.0366$ ) and acetonitrile ( $N=74$ ,  $SD=0.0438$ ) where  $N$  is the number of data points, that is ions plus nonelectrolytes, and  $SD$  is the standard deviation in  $\log_{10}(D^0)$ . It is shown that solute hydrogen bond acidity, solute hydrogen bond basicity and solute volume all lower the diffusion constants of ions and nonelectrolytes in the various solvents studied.

**Keywords** Ions · Nonelectrolytes · Diffusion coefficients · Linear free energy relationship · Hydrogen bond acidity · Hydrogen bond basicity

## 1 Introduction

Diffusion coefficients of solutes in water and in organic solvents play a very important role in chemical engineering [1], environmental chemistry [2] and in biological chemistry [3]. Therefore it is not surprising that there have been numerous studies on the correlation and prediction of limiting diffusion coefficients, mostly diffusion coefficients in water but also

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in organic solvents [4]. Many of the older studies on diffusion coefficients have involved a restricted number of solutes, but recently there have been a number of studies which dealt with much larger numbers of solutes. Gharagheizi and Sattari [5] used a data base of diffusion coefficients in water for 300 solutes. They calculated 1664 descriptors for each solute from the Dragon software [6], and reduced these to the best six descriptors to use in a linear equation. Garagheizi et al. [7] later used a huge data base of 4852 solutes to develop a predictive method based on 148 functional groups. Unfortunately, although they give the predicted diffusion coefficients for all 4852 solutes, the authors do not give any actual experimental values. Garagheizi [8] later used the 4852 data base to obtain a linear three parameter equation using descriptors calculated from the Dragon software program.

Use of extensive data bases has not been confined to diffusion coefficients in water. Magalhaes et al. [9] studied 3463 values of diffusion coefficients in water and in organic solvents. However, since 18 solvents were examined, the number of solutes per solvent is not that large. Li et al. [10] used a linear free energy relationship based on the Abraham equation [11], to correlate 743 diffusion coefficients in 25 solvents; again, although a large number of data points was used, the number per solvent is still rather limited.

All these recent studies involve only nonelectrolytes as solutes. Ions and ionic species are excluded. Indeed it seems impossible for methods based on the calculation of Dragon descriptors or on functional group analysis to be extended to ionic molecules. The only study of limiting diffusion coefficients that included ions and ionic molecules has been our own work on solutes in water [12]. It is the aim of the present work to enlarge the data base of ionic and nonelectrolyte solutes in water, and to extend our analysis to as many organic solvents for which data on nonelectrolytes, ions and ionic species are available.

## 2 Methods

Our general method is based on the linear free energy equation, LFER, Eq. 1.

$$\log_{10}(D^{\circ}) = c + e \cdot E + s \cdot S + a \cdot A + b \cdot B + v \cdot V + j^{+} \cdot J^{+} + j^{-} \cdot J^{-} \quad (1)$$

The dependent variable is  $\log_{10}(D^{\circ})$ , where  $D^{\circ}$  is the diffusion coefficient at infinite dilution at 298 K for a series of solutes in a given solvent. The independent variables in Eq. 1 ( $E$ ,  $S$ ,  $A$ ,  $B$ ,  $V$ ,  $J^{+}$  and  $J^{-}$ ) are properties or descriptors of the solutes and the coefficients ( $c$ ,  $e$ ,  $s$ ,  $a$ ,  $b$ ,  $v$ ,  $j^{+}$  and  $j^{-}$ ) are the complementary properties of the solvent system. Solute and solvent properties have been described in detail in earlier publications [13–21], there are several reviews on our method [22–24], and a number of applications [25–27] and so only an outline will be given here.  $E$  is the solute excess molar refraction in  $\text{cm}^3 \cdot \text{mol}^{-1}/10$ ,  $S$  is a measure of the solute polarity/polarizability,  $A$  and  $B$  refer to the hydrogen bond acidity and hydrogen bond basicity of the solute, and  $V$  is McGowan's characteristic molecular volume of the solute in  $\text{cm}^3 \cdot \text{mol}^{-1}/100$  [28].  $J^{+}$  and  $J^{-}$  are properties of positively charged and negatively charged solutes. Note that for positively charged solutes  $J^{-} = 0$ , for negatively charged solutes  $J^{+} = 0$ , and for nonelectrolytes  $J^{+} = J^{-} = 0$ . For the specific case of zwitterionic aminoacid solutes both  $J^{+}$  and  $J^{-}$  are necessary to characterize the solutes [29].

### 3 Results

Diffusion coefficients for ions and ionic species in organic solvents were obtained from data on single-ion conductances  $A_i^0$  through the Nernst–Einstein equation, Eq. 2, where  $F$  is the Faraday constant. We give diffusion coefficients for ions and nonelectrolytes in units of  $10^{-5} \text{ cm}^2 \cdot \text{s}^{-1}$  at 298 K.

$$D_i^0 = \frac{RT}{F^2} A_i^0 \quad (2)$$

#### 3.1 Water

Data for ions and ionic species were those that we used before [12]. For nonelectrolytes we supplemented our previous data with a considerable number of extra values of  $\log_{10}(D^0)$  [2, 5, 7, 30–34], leading to a total of 377 values, including ions, ionic species, zwitterionic amino acids and neutral nonelectrolytes. The list of solutes, diffusion coefficients and solute descriptors are given in Table S1 of the Supplementary Material. We found that polyaromatic hydrocarbons with three or more condensed rings were systematically out of line, and we included an indicator variable for these solutes,  $I_{\text{pha}}$ , that has the value  $I_{\text{pha}}=1$  for the condensed ring compounds and  $I_{\text{pha}}=0$  for all other solutes. Our final equation is

$$\log_{10}(D^0) = 0.1803 - 0.0119E + 0.0319S + 0.0104A - 0.0362 \\ - 0.2519V - 0.0148J^+ + 0.0205J^- - 0.0798I_{\text{pha}} \quad (3)$$

$N=377$ ,  $SD=0.0474$ ,  $R^2=0.840$ ,  $F=241.20$ ,  $PRESS=0.91821$ ,  $Q^2=0.823$ , and  $PSD=0.0499$ .

Here and elsewhere,  $N$  is the number of data points (solute),  $SD$  is the standard deviation,  $R$  is the equation correlation coefficient,  $F$  is the Fisher  $F$ -statistic and  $PRESS$  and  $Q^2$  are the leave-one-out statistics. We use the predictive standard deviation,  $PSD$ , as a measure of the predictive capability of the equation [35] rather than the method of division into test and training sets, because  $PSD$  is based on the leave-one-out statistics, it takes into account the number of data points and the number of descriptors and it uses data on all the data points. The high value of the leave-one-out  $Q^2$  shows that the equation is statistically sound.

#### 3.2 Ethanol

We obtained diffusion coefficients for ions from conductance data through Eq. 2 [36–38]. We took our previous data on nonelectrolytes [12] and added further data [39–42] to give a total of 96 values for ions plus nonelectrolytes. The resulting equation for  $\log_{10}(D^0)$  is Eq. 4. The term in  $I_{\text{pha}}$  was not significant. Both the value of  $Q^2$  and  $PSD$  show that the equation is statistically sound. The list of solutes, diffusion coefficients and solute descriptors are given in Table S2.

$$\log_{10}(D^0) = 0.3710 - 0.1058E + 0.1369S - 0.3189A - 0.1629 \\ - 0.2215V + 0.4084J^+ + 0.1096J^- \quad (4)$$

$N=96$ ,  $SD=0.0666$ ,  $R^2=0.932$ ,  $F=169.17$ ,  $PRESS=0.58308$ ,  $Q^2=0.897$ , and  $PSD=0.0823$ .

### 3.3 Methanol

There are numerous studies on single ion conductance in methanol (43–47, 48) from which we derived corresponding diffusion coefficients. Diffusion coefficients of nonelectrolytes have been well studied (4, 10, 34, 39–42, 49–53) and we collected data on a total of 96 solutes, ionic plus nonelectrolytes, that yielded Eq. 5. The list of solutes, diffusion coefficients and solute descriptors are given in Table S3.

$$\log_{10}(D^0) = 0.4601 + 0.0197E - 0.0020S - 0.2403A - 0.0463 \\ - 0.1377V + 0.0252J^+ - 0.0788J^- \quad (5)$$

$N=96$ ,  $SD=0.0332$ ,  $R^2=0.915$ ,  $F=135.98$ ,  $PRESS=0.1232$ ,  $Q^2=0.893$ , and  $PSD=0.0374$ .

### 3.4 Propan-1-ol

Diffusion coefficients for ions were obtained from conductance data through Eq. 2 [30, 37, 43, 45]. There is surprisingly little data on diffusion coefficients of nonelectrolytes [4, 34], not enough to enable us to obtain a robust equation based on Eq. 1. However, there are considerable data on nonelectrolytes in octanol [3, 49, 50] as well as in methanol and ethanol (see above). For any given solute, a plot of  $\log_{10}(D^0)$  against the number of carbon atoms in the alcohol is almost linear. Taking into account the slight nonlinearity, it is then quite easy to interpolate values of  $\log_{10}(D^0)$  to obtain estimates in propan-1-ol (and in butan-1-ol). We obtained a total of 73 values of  $\log_{10}(D^0)$  for ions and nonelectrolytes that yielded Eq. 6. The list of solutes, diffusion coefficients and solute descriptors are given in Table S4.

$$\log_{10}(D^0) = 0.1263 - 0.0353E - 0.0144S - 0.4433A - 0.1063 \\ - 0.0938V - 0.1097J^+ - 0.2016J^- \quad (6)$$

$N=71$ ,  $SD=0.0487$ ,  $R^2=0.948$ ,  $F=164.81$ ,  $PRESS=0.20879$ ,  $Q^2=0.928$ , and  $PSD=0.0576$ .

### 3.5 Butan-1-ol

Data are available for ions [30, 45], but, again, there is a lack of data on nonelectrolytes [4, 10, 39, 40, 42, 47]. We adopted the same stratagem as for propan-1-ol solvent and obtained data on a total of 53 solutes, leading to Eq. 7. The list of solutes, diffusion coefficients and solute descriptors are given in Table S5.

$$\log_{10}(D^0) = 0.0608 - 0.0036E - 0.0316S - 0.4993A - 0.0461 \\ - 0.1822V - 0.1777J^+ - 0.2422J^- \quad (7)$$

$N=53$ ,  $SD=0.0600$ ,  $R^2=0.926$ ,  $F=80.29$ ,  $PRESS=0.32266$ ,  $Q^2=0.852$ , and  $PSD=0.0846$ .

### 3.6 Octan-1-ol

Diffusion coefficients for ions are available from conductance data [46, 54] and there is just enough data on diffusion coefficients for nonelectrolytes [3, 10, 54–57] to be able to construct Eq. 8 for a total of 61 solutes. The list of solutes, diffusion coefficients and solute descriptors are given in Table S6.

$$\log_{10}(D^0) = -0.1233 - 0.0382E - 0.0440S - 0.5710A - 0.2862 \\ - 0.2378V - 0.8020J^+ - 0.2899J^- \quad (8)$$

N=61, SD=0.0684, R<sup>2</sup>=0.949, F=141.41, PRESS=0.3327, Q<sup>2</sup>=0.932, and PSD=0.0792.

### 3.7 Propanone

There is a reasonable amount of data on the conductance of ions in propanone [46, 58], and several studies on the diffusion of nonelectrolytes [10, 50, 59–63]. We did not use the results of Hejtmánek and Schnelder [63] on crown ethers that were completely out of line. Interestingly, these experimental results were not well reproduced by any of the predictive methods used [63]. We compiled a total of 86 values of log<sub>10</sub>(D<sup>0</sup>) including ions and nonelectrolytes, that yielded Eq. 9. The list of solutes, diffusion coefficients and solute descriptors are given in Table S7.

$$\log_{10}(D^0) = 0.6593 - 0.0221E - 0.0162S - 0.1718A - 0.0031 \\ - 0.1102V - 0.0167J^+ - 0.0631J^- \quad (9)$$

N=86, SD=0.0366, R<sup>2</sup>=0.837, F=57.37, PRESS=0.14773, Q<sup>2</sup>=0.767, and PSD=0.0435.

### 3.8 Acetonitrile

There have been a several studies on conductance of ions in acetonitrile solvent [44, 46, 58, 64–67] so that we were able to obtain log<sub>10</sub>(D<sup>0</sup>) for 18 ions. There are also a considerable number of studies on nonelectrolytes [10, 40, 68–74] so that we had a combined total of 74 log<sub>10</sub>(D<sup>0</sup>) values for ions and nonelectrolytes. This led to Eq. 10. The list of solutes, diffusion coefficients and solute descriptors are given in Table S8.

$$\log_{10}(D^0) = 0.6612 - 0.0283E - 0.0126S - 0.2311A - 0.0511 \\ - 0.1399V + 0.034J^+ - 0.0287J^- \quad (10)$$

N=74, SD=0.0438, R<sup>2</sup>=0.886, F=73.53, PRESS=0.15983, Q<sup>2</sup>=0.857, and PSD=0.0492.

## 4 Discussion

There are several more solvents than those we have studied for which conductance data exists for a sufficient number of ions to be able to use in Eq. 1. Unfortunately there are not enough data on nonelectrolytes in these solvents to obtain statistically meaningful

**Table 1** Minimum and maximum values of the independent variables used in Eq. 1 for nonelectrolytes

Descriptor	Solvent butan-1-ol		Solvent water	
	Minimum	Maximum	Minimum	Maximum
<i>E</i>	0.00	1.67	−0.31	3.03
<i>S</i>	0.00	2.10	−0.21	2.78
<i>A</i>	0.00	1.09	0.00	3.00
<i>B</i>	0.00	2.73	0.00	3.05
<i>V</i>	0.25	3.63	0.27	2.73

equations. On the other hand, there are a large number of nonpolar solvents for which  $\log_{10}(D^0)$  are available, but for which there is no data, or very little data, on  $\log_{10}(D^0)$  for ions. However, we have results for enough solvents to show that Eq. 1 can be regarded as a general equation for the correlation and prediction of diffusion coefficients of ions and nonelectrolytes in water and in organic solvents. We include diffusion coefficients of zwitterionic aminoacids (in water), of the tetraalkyltins (in most of the solvents) and of the inorganic complexes  $\text{Fe}(\text{acac})_3$  and  $\text{Co}(\text{acac})_3$  as well as a number of ferrocenes (in acetonitrile) so that the scope of our equations is very large indeed. The generality of our equations is not limited by functional groups, but depends on the range of the independent variables in the various equations. We give in Table 1 the maximum and minimum values of the independent variables for the nonelectrolytes studied with water and butan-1-ol solvents; that is, the solvents with the largest and smallest numbers of the diffusion coefficients. Even for butan-1-ol, the range of the independent variables for nonelectrolytes is large enough to include a very wide range of solute types. The statistics of our equations for  $\log_{10}(D^0)$  are all quite good, with SD values ranging from 0.0332 (methanol) to 0.0684 (octan-1-ol). By comparison, our present equation for solvent water has  $\text{SD}=0.0474$  for 377 ions plus nonelectrolytes as compared to our previous statistic [12] of  $\text{SD}=0.085$  for 190 ions plus nonelectrolytes in water.

We have data on diffusion coefficients for the large ions  $\text{Ph}_4\text{As}^+$ ,  $\text{Ph}_4\text{P}^+$  and  $\text{Ph}_4\text{B}^-$  but in several solvents the observed values of  $\log_{10}(D^0)$  were considerably out of line and we then omitted these ions from all of our analyses. We have no explanation for this observation. Our descriptors for these ions have been used on several occasions in partition systems with good results [24] so errors in the descriptors can be ruled out. Our calculated  $\log_{10}(D^0)$  values for  $\text{Ph}_4\text{As}^+$  and  $\text{Ph}_4\text{P}^+$  were always quite close to the calculated value for  $\text{Ph}_4\text{B}^-$  as is required by the TATB convention [75, 76] that we used to obtain data on single

**Table 2** Summary of coefficients in Eq. 1

Solvent	<i>c</i>	<i>e</i>	<i>s</i>	<i>a</i>	<i>b</i>	<i>v</i>	<i>j</i> <sup>+</sup>	<i>j</i> <sup>−</sup>
Water	0.1752	−0.0066	0.0373	0.0015	−0.0348	−0.2526	−0.0112	0.0109
Methanol	0.4601	0.0197	−0.0020	−0.2403	−0.0463	−0.1377	0.0252	−0.0788
Ethanol	0.3710	−0.1058	0.1369	−0.3189	−0.1629	−0.2215	0.4084	0.1096
Propan-1-ol	0.1263	−0.0353	−0.0144	−0.4433	−0.1063	−0.0938	−0.1097	−0.2016
Butan-1-ol	0.0608	−0.0036	−0.0316	−0.4993	−0.0461	−0.1822	−0.1777	−0.2422
Octan-1-ol	−0.1233	−0.0382	−0.0440	−0.5710	−0.2862	−0.2378	−0.8020	−0.2899
Propanone	0.6593	−0.0221	−0.0162	−0.1718	−0.0031	−0.1102	−0.0167	−0.0631
Acetonitrile	0.6612	−0.0283	−0.0126	−0.2311	−0.0511	−0.1399	0.0340	−0.0287

ions [24], so that the  $\log_{10}(D^0)$  values we use for single ions are compatible with the TATB convention that we use to obtain descriptors for single ions.

It is useful to compare the coefficients in Eq. 1 for the various solvents that we have studied, and these are collected in Table 2. The three most important terms for both ions and nonelectrolytes are  $a \cdot A$ ,  $b \cdot B$  and  $v \cdot V$  with the  $a$ -,  $b$ - and  $v$ -coefficients all being negative. Thus increase in solute hydrogen bond acidity, hydrogen bond basicity and volume all lead to a decrease in the limiting diffusion coefficient, the effect of solute volume on diffusion being well known [77, 78]. The decrease in diffusion due to increase in solute hydrogen bond acidity and hydrogen bond basicity can probably be attributed to increases in solute–solvent acid–base interactions. It would be useful if the coefficients in Table 2 could be used to predict coefficients for other solvents. We examined the coefficients for water and the alcohols as a function of the number of carbon atoms in the solvents. Although there are some general trends, we were unable to find statistically satisfactory correlations between any of the coefficients and the number of carbon atoms. It can be seen, almost by inspection, that the coefficients in water and in ethanol are often outliers to the general trends.

## 5 Conclusions

We have now shown that it is possible to correlate limiting diffusion coefficients for nonelectrolytes, ions and ionic species in water and in seven organic solvents with Abraham descriptors through the linear free energy equation, LFER, Eq. 1. We can therefore now regard Eq. 1 as a general equation for the correlation of limiting diffusion coefficients. In principle, it could be applied to any solvent for which diffusion data exists on nonelectrolytes, ions and ionic species. Of course, this excludes non-polar solvents where diffusion data are restricted to nonelectrolytes, but there are numerous polar or semi-polar solvents to which Eq. 1 could apply. We have not been able to extend our studies to additional solvents simply because of the lack of data on either nonelectrolytes or ionic species. Conductance data exists for ions in 2-methoxyethanol [79, 80], in *N,N*-dimethylformamide [66, 81] and in formic acid [82], and these could be used to obtain corresponding limiting diffusion coefficients through Eq. 2. However, there is not enough data on nonelectrolytes in these solvents to apply Eq. 1. Whether Eq. 1 could be applied to diffusion of nonelectrolytes and ions through biological or other membranes [3] remains to be seen.

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