# Densities of Sodium Tetrafluoroborate Aqueous Solutions at 20°C

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## Abstract

Densities of solutions of $NaBF_4$ in $H_2O$ have been determined at 20.0°C over the concentration range 0.05 to 9.0 molal (0 to 50 wt %) $NaBF_4$. The results are represented by D (g/mL, 20°C) = $9.726x10^{-5}m^3$ - $3.2157x10^{-3}m^2$ + $6.7447x10^{-2}m$ + 0.99843, where D is density and m is molality. This equation was used to derive concentrative properties for $NaBF_4$ solutions. The raw density data were used to derive partial molal volumes. The partial molal volume at infinite dilution is 37.6 ± 2.7 mL/mol at 20°C. The partial molal volume at 20°C is represented by $\bar{v}_2 = 37.5 + 9.22m^{1/2} - 2.92m$ from 0 to 2.5 m $NaBF_4$ and $\bar{v}_2 = 44.6 + 0.081m$ from 2.5 to 9 m $NaBF_4$.

Analytical data and plant solution compositions are often reported in molarity units. Densities of salt solutions are needed to convert the concentrations to molal basis in order to utilize physical property data that have been established on a molal basis, for example, solution reaction equilibrium constants or activity coefficients. We report here the densities at 20.0°C of sodium tetrafluoroborate ($NaBF_4$) solutions from 0.05 molal to 9.0 molal, near saturation of 9.2 molal.

**Experimental**

Sodium tetrafluoroborate, 98 %, Chemical Abstracts Service Registry Number 13755-29-8, an off-grey solid obtained from ACROS, was purified by recrystallization from water, according to the procedure of Platford.[1] The $NaBF_4$ (125.8 g) was added to 60 mL of hot Millipore water to dissolve it. The cooled solution was separated from the precipitated crystals by suction filtration. A black solid deposited on the surface of the filter paper and white $NaBF_4$ crystals were on top of them. The white crystals (74.1 g, 59% recovery) were physically separated from the mixture of black solid and white crystals. This $NaBF_4$ was dried to a constant weight in a drying oven at 120°C and stored in a desiccator until use.

Solutions of $NaBF_4$ were prepared by weighing the dried crystals and adding degassed Millipore $H_2O$ by weight. Masses were determined on an analytical balance of 0.1 mg sensitivity that was calibrated against NIST-traceable standard weights and were corrected for air bouyancy. The $NaBF_4$ masses ranged from 0.28 g to 5.93 g in 50 to 6.0 g of $H_2O$, respectively. Thus, the solution molal concentrations were measured to an accuracy of 0.04% at the lowest concentration to 0.003% at the highest concentration. The individual solution concentration uncertainties are reported with the results.

Densities were determined with an Anton Parr DNA 4500 oscillating U-tube density meter.[2] The technical specification for standard deviation in repeatability is stated to be 0.00001 g/cm$^3$. Sources and magnitudes of error are discussed by Fitzgerald for the Anton Paar DMA 5000 density meter.[3] For solutions with a limited viscosity range of less than 30 mPa•s, the maximum error is less than 0.000015 g/cm$^3$. The DMA 5000 has a technical specification for standard deviation in repeatability of $1\times10^{-6}$ g/cm$^3$, an order of magnitude less than for the DMA 4500. Thus, a maximum error for the DMA 4500 of approximately 0.00015 g/cm$^3$ might be conservatively assumed (less than 0.015% for the current measurements). The following precisions reflect actual measurement variabilities, which are slightly greater than these best possible specifications.

Three measurements were taken at each concentration and averaged for solutions up to 1.5 molal $NaBF_4$ and two measurements were averaged for higher concentrations. The maximum variability of an individual measurement from the average was 0.02% or less for all but one of the 23 data points, which had a maximum variability of 0.04%. The average standard deviation of measurements was 0.00016 g/mL (0.013%). The instrument calibration was checked with boiled (degassed) Millipore $H_2O$ (<18 MOhms) (density at 20°C, 0.998204 g/mL)[4, 5] after each series of measurements at a concentration. The calibration correction thus determined started at -0.01% and gradually changed in a regular fashion to +0.13% as the measurements progressed from the lowest concentration to the highest

in order. This may be due to a slight corrosion of the cell by the $NaBF_4$ solutions. The calibration corrections are considered to be good to 0.01% of the measured value.

The results of the instrument were checked by determining the densities of the nominal 1.0 and 9.0 molal $NaBF_4$ solutions from the mass of solution contained in a 10 mL Gay-Lussac specific gravity bottle at 20.00°C and by measuring the mass of solution delivered from a 1 mL pipet. The volumes of the bottle and pipet were calibrated with water (standard deviation of 5 measurements, 0.003% for the bottle and 0.025% for the pipet). Five determinations were made by each method for each solution, except that only one measurement was made on the 9 molal solution with the specific gravity bottle. The results agreed with the density meter measurements within 0.04% in all cases as follows: 1 m $NaBF_4$ (pipet 0.01% difference, standard deviation 0.06%; specific gravity bottle 0.04% difference, standard deviation 0.03%); 9 m $NaBF_4$ (pipet 0.02% difference, standard deviation 0.09%; specific gravity bottle 0.02% difference, single point). In all cases, the density meter read higher than the others. These results validate the density meter measurements that are used in the analysis and data reduction.

Temperature (ITS-90) was controlled and measured to within 0.01°C with two integrated NIST-traceable 100 ohm platinum resistance thermometers. The temperature was controlled to 20.00±0.01°C. This corresponds to an uncertainty in density of ±0.0002%.

The overall uncertainty in the averaged density measurements is judged to be less than 0.03%, based on the pooling of 2 times the average standard deviation of measurement (0.02%) and 2 times the estimated error of calibration correction (0.02%). The combined uncertainties in individual measurements of molality and density (pooled) are less than 0.05% at the lowest concentration to less than 0.03% at the highest concentration.

**Results**

The experimental data are summarized in Table 1. Including the 0 molal data point of 0.99820 g/mL, the data are well fitted by the equation

$$D\ (g/mL, 20°C) = 9.726x10^{-5}m^3 - 3.2157x10^{-3}m^2 + 6.7447x10^{-2}m + 0.99843,\ R^2 = 0.99997$$

where m is molality and D is density. This equation was used to derive concentrative properties for $NaBF_4$ solutions in tabular form (see Table 2) identical to those provided for solutions in the CRC Handbook of Chemistry and Physics.[6] The heading notations are identical to the CRC Handbook:

$\rho$ = density, g/mL

$D_{20}^{20}$ = specific gravity at 20°C = $D_4^{20} / 0.99823$

$C_s$ = $NaBF_4$ concentration, g/L

M = molar concentration, g-mol/L

$C_w$ = total water concentration, g/L

$(C_0 - C_w)$ = water displaced by anhydrous solute, g/L

Partial molal volumes were determined from the density data as follows. The apparent molal volume, ${}^{\phi}V$, was first derived from the raw density values:[7]

$$ {}^{\phi}V = \left[ \frac{1000}{mdd_0}(d_0 - d) + \frac{M_2}{d} \right] \quad (1) $$

where $d_0$ is the solvent ($H_2O$) density, 0.998204 g/mL at 20°C, and $M_2$ is the molecular weight of the solute $NaBF_4$, 109.794 g/mol. Extrapolation of the apparent molal volume to infinite dilution yielded ${}^{\phi}V^0$, the value of ${}^{\phi}V$ at infinite dilution, of 37.6 mL/mol. This is also the value of partial molal volume of $NaBF_4$ at infinite dilution, $\bar{v}_2^0$.[7]

As discussed above, uncertainty in individual density values is estimated to be approximately 0.05%. The corresponding uncertainty in ${}^{\phi}V$ is obtained[7] by differentiating equation (1) with respect to d, yielding a probable error in ${}^{\phi}V$ of

$$ \left( \frac{-1000}{m} + M_2 \right) \frac{\delta d}{d^2} $$

This would correspond to an uncertainty in apparent molal volume at the lower limit of 0.05 m $NaBF_4$ of 26% (±9.9 mL/mol). However, based on the uniformity of the series of density values and the good extrapolation to the infinitely dilute value of 0.9982 g/mL, the associated uncertainty for the extrapolated apparent molal volume is judged to be approximately 7% (±2.7 ml/mol), corresponding to ±0.014% uncertainty in density.

In order to represent the apparent molal volumes analytically, two regions of data were fitted in overlapping ranges. The data from 0 to 6 molal $NaBF_4$ were fitted to the Redlich-Meyer function[7, 8] to yield a function suitable to 2.5 molal. To obtain a suitable function above 2.5 molal, the data from 1 to 9 molal were fitted to a quadratic function.

Partial molal volume values, $\bar{v}_2$, were then derived from these functions using the relationship[7, 9]

$$ \bar{v}_2 = {}^{\phi}V + m \frac{\partial {}^{\phi}V}{\partial m} $$

The quadratic partial molal volume equation had a slight maximum at 8 molal $NaBF_4$. Considering that the actual values would continue a slight increase, an adequate representation above 2.5 molal was obtained by fitting a linear function to the two points of the 2.5 molal value from the Redlich Meyer equation and the 8 molal value from the

quadratic equation. This approach yielded a smooth transition between equations. The resulting representation of the partial molal volume (mL/mol at 20°C) is, thus,

$$\bar{v}_2 = 37.5 + 9.22m^{1/2} - 2.92m \quad \text{from 0 to 2.5 m } NaBF_4$$

and

$$\bar{v}_2 = 44.6 + 0.081m \quad \text{from 2.5 to 9 m } NaBF_4$$

Considering variability in individual values and the inaccuracies of the fitted equations, the uncertainty in individual calculated values is approximately ±2.7 mL/mol at the lower end of the concentration range and ±1 mL/mol at the upper end.

**Literature Cited**

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Table 1. Experimental Values of $NaBF_4$ Solution Densities at 20.00°C

| $NaBF_4$ Concentration, molal | Uncertainty in Concentration,[a] molal | Density, g/mL | Uncertainty in Density,[b] g/mL |
|---|---|---|---|
| 0.05018 | 0.00002 | 1.0018 | 0.0003 |
| 0.10020 | 0.00002 | 1.0053 | 0.0003 |
| 0.19960 | 0.00004 | 1.0121 | 0.0003 |
| 0.29953 | 0.00004 | 1.0186 | 0.0003 |
| 0.39971 | 0.00004 | 1.0252 | 0.0003 |
| 0.49934 | 0.00004 | 1.0316 | 0.0003 |
| 0.99611 | 0.00004 | 1.0629 | 0.0003 |
| 1.4947 | 0.0002 | 1.0915 | 0.0003 |
| 1.9909 | 0.0002 | 1.1187 | 0.0003 |
| 2.4885 | 0.0002 | 1.1485 | 0.0003 |
| 2.9927 | 0.0002 | 1.1744 | 0.0003 |
| 3.4955 | 0.0002 | 1.1995 | 0.0003 |
| 4.0035 | 0.0002 | 1.2232 | 0.0003 |
| 4.4898 | 0.0002 | 1.2462 | 0.0003 |
| 4.9857 | 0.0002 | 1.2670 | 0.0003 |
| 5.4797 | 0.0002 | 1.2881 | 0.0003 |
| 5.9982 | 0.0003 | 1.3090 | 0.0003 |
| 6.4785 | 0.0003 | 1.3244 | 0.0003 |
| 6.9477 | 0.0003 | 1.3437 | 0.0003 |
| 7.4944 | 0.0003 | 1.3648 | 0.0003 |
| 7.9971 | 0.0003 | 1.3822 | 0.0003 |
| 8.4896 | 0.0003 | 1.3991 | 0.0003 |
| 8.9823 | 0.0003 | 1.4152 | 0.0003 |

[a]Based on 0.0001 g uncertainty in measured masses of $NaBF_4$ and $H_2O$.

[b]Based on the pooled errors of 2 times average standard deviation of measurement and 2 times the estimated error of instrument calibration correction.

Table 2. Concentrative Properties of $NaBF_4$ Aqueous Solutions at 20°C.

| $NaBF_4$ % by wt. | ρ, g/mL | $D_{20}^{20}$ | $C_s$ g/L | M g-mol/L | $C_w$ g/L | $(C_0 - C_w)$ g/L |
|---|---|---|---|---|---|---|
| 0.50 | 1.0014 | 1.0031 | 5.007 | 0.04560 | 996.4 | 1.9 |
| 1.00 | 1.0045 | 1.0063 | 10.05 | 0.09149 | 994.5 | 3.8 |
| 1.50 | 1.0077 | 1.0095 | 15.12 | 0.1377 | 992.6 | 5.7 |
| 2.00 | 1.0109 | 1.0127 | 20.22 | 0.1841 | 990.7 | 7.6 |
| 2.50 | 1.0141 | 1.0159 | 25.35 | 0.2309 | 988.8 | 9.5 |
| 3.00 | 1.0173 | 1.0191 | 30.52 | 0.2780 | 986.8 | 11.5 |
| 3.50 | 1.0206 | 1.0224 | 35.72 | 0.3253 | 984.8 | 13.5 |
| 4.00 | 1.0238 | 1.0256 | 40.95 | 0.3730 | 982.9 | 15.4 |
| 4.50 | 1.0271 | 1.0289 | 46.22 | 0.4209 | 980.8 | 17.5 |
| 5.00 | 1.0303 | 1.0322 | 51.52 | 0.4692 | 978.8 | 19.5 |
| 5.50 | 1.0336 | 1.0355 | 56.85 | 0.5178 | 976.8 | 21.5 |
| 6.00 | 1.0369 | 1.0388 | 62.22 | 0.5667 | 974.7 | 23.6 |
| 6.50 | 1.0402 | 1.0421 | 67.62 | 0.6158 | 972.6 | 25.7 |
| 7.00 | 1.0436 | 1.0454 | 73.05 | 0.6653 | 970.5 | 27.8 |
| 7.50 | 1.0469 | 1.0488 | 78.52 | 0.7151 | 968.4 | 29.9 |
| 8.00 | 1.0503 | 1.0521 | 84.02 | 0.7653 | 966.3 | 32.0 |
| 8.50 | 1.0536 | 1.0555 | 89.56 | 0.8157 | 964.1 | 34.2 |
| 9.00 | 1.0571 | 1.0589 | 95.13 | 0.8665 | 961.9 | 36.4 |
| 9.50 | 1.0605 | 1.0623 | 100.74 | 0.9176 | 959.7 | 38.6 |
| 10.00 | 1.0639 | 1.0658 | 106.39 | 0.9690 | 957.5 | 40.8 |
| 11.00 | 1.0708 | 1.0727 | 117.79 | 1.0728 | 953.0 | 45.3 |
| 12.00 | 1.0778 | 1.0797 | 129.33 | 1.1780 | 948.4 | 49.9 |
| 13.00 | 1.0848 | 1.0868 | 141.03 | 1.2845 | 943.8 | 54.5 |
| 14.00 | 1.0920 | 1.0939 | 152.87 | 1.3924 | 939.1 | 59.2 |
| 15.00 | 1.0991 | 1.1011 | 164.9 | 1.5017 | 934.3 | 64.0 |
| 16.00 | 1.1065 | 1.1084 | 177.0 | 1.6124 | 929.4 | 68.9 |
| 17.00 | 1.1138 | 1.1158 | 189.4 | 1.7246 | 924.5 | 73.8 |
| 18.00 | 1.1213 | 1.1233 | 201.8 | 1.8383 | 919.5 | 78.8 |
| 19.00 | 1.1288 | 1.1308 | 214.5 | 1.9534 | 914.3 | 83.9 |
| 20.00 | 1.1365 | 1.1385 | 227.3 | 2.0702 | 909.2 | 89.1 |
| 22.00 | 1.1520 | 1.1540 | 253.4 | 2.3083 | 898.6 | 99.7 |
| 24.00 | 1.1679 | 1.1700 | 280.3 | 2.5530 | 887.6 | 110.7 |
| 26.00 | 1.1843 | 1.1864 | 307.9 | 2.8044 | 876.4 | 121.9 |
| 28.00 | 1.2010 | 1.2031 | 336.3 | 3.0629 | 864.7 | 133.6 |
| 30.00 | 1.2182 | 1.2204 | 365.5 | 3.3286 | 852.8 | 145.5 |
| 32.00 | 1.2359 | 1.2381 | 395.5 | 3.6020 | 840.4 | 157.9 |
| 34.00 | 1.2540 | 1.2562 | 426.4 | 3.8833 | 827.7 | 170.6 |
| 36.00 | 1.2727 | 1.2749 | 458.2 | 4.1729 | 814.5 | 183.8 |
| 38.00 | 1.2918 | 1.2941 | 490.9 | 4.4710 | 800.9 | 197.4 |
| 40.00 | 1.3115 | 1.3138 | 524.6 | 4.7780 | 786.9 | 211.4 |
| 42.00 | 1.3317 | 1.3341 | 559.3 | 5.0943 | 772.4 | 225.9 |
| 44.00 | 1.3526 | 1.3549 | 595.1 | 5.4203 | 757.4 | 240.9 |
| 46.00 | 1.3740 | 1.3764 | 632.0 | 5.7564 | 741.9 | 256.4 |
| 48.00 | 1.3960 | 1.3984 | 670.1 | 6.1029 | 725.9 | 272.4 |
| 50.00 | 1.4186 | 1.4211 | 709.3 | 6.4603 | 709.3 | 289.0 |