kcal mol^{-1} for four other isomers. The magnitude of the differences for the 75 liquid decanes is as follows: less than 0.20 kcal mol^{-1} for 44 isomeric decanes, 0.2–0.4 kcal mol^{-1} for 16 decanes, 0.4–1.0 kcal mol^{-1} for 4 isomers, and 1.2–4.9 kcal mol^{-1} for 11 other isomers. Since the experimental uncertainty in any one of these values is at least ± 0.2 kcal mol^{-1}, the calculated property values for nonanes and decanes are considered as reliable as the experimental and are recommended for general use. It is also important to note that the generalized trigonal additivity procedure is the most accurate of all procedures developed thus far for the correlation of the thermodynamic properties of the alkanes.

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Activity and Osmotic Coefficients in Dilute Aqueous Solutions of Bi-Univalent Electrolytes at 25 °C

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In nonassociative dilute aqueous electrolyte solutions, the Stokes and Robinson equation reduces to a simpler form, $\log \gamma_\pm = \log f_{\pm,\mathrm{DH}} + 0.0156(h - \nu/2)m$, where $f_{\pm,\mathrm{DH}}$ is the mean rational activity coefficient calculated from the Debye–Hückel equation. Thus the mean molal activity coefficients of an electrolyte in dilute regions can be calculated from the equation if suitable values of $\mathring{a}$ and h are available. The molal osmotic coefficients of a solution are related to the activity coefficients by means of the Gibbs–Duhem relation. A simple equation for calculating osmotic coefficients is derived; it takes the form $\phi = \phi_{\mathrm{DH}} + 0.018hm$ where ϕ_{DH} is the molal osmotic coefficient of the solution calculated from the Debye–Hückel equation by use of the Gibbs–Duhem relation. These equations are applied to calculate the activity and osmotic coefficients in dilute aqueous solutions of some bi-univalent electrolytes, including chlorides, bromides, and perchlorates, concentration up to 0.1 m.

Hamer and Wu (*2*) have recently compiled numerous data of osmotic and activity coefficients in dilute solutions of 1–1 electrolytes. However, these coefficients for other types of electrolytes in dilute regions are lacking in general. When the experimental data in more dilute regions are not available, they can be derived directly from equations containing parameters which are obtained experimentally at higher concentration regions. A method based on the Stokes–Robinson hydration model (*4, 6*) is proposed to solve this problem. Activity and osmotic coefficients in solutions of some 2–1 electrolytes are calculated and compiled in this communication.

In nonassociated dilute electrolyte solutions the Stokes–Robinson two-parameter equation reduces to a simpler form (*4*), i.e.

$$\log \gamma_\pm = \log f_{\pm,\mathrm{DH}} + 0.0156(h - \nu/2)m \qquad (1)$$

or

$$\ln \gamma_\pm = \ln f_{\pm,\mathrm{DH}} + 0.036(h - \nu/2)m \qquad (2)$$

in which $\gamma_\pm$ is the mean molal activity coefficient, $f_{\pm,\mathrm{DH}}$ is the mean rational activity coefficient calculated from the Debye–Hückel equation, h is the hydration number, ν is the stoichiometric ion number of the electrolyte, and m is the molality of the solution. The Debye–Hückel equation (*5*) is

$$\log f_{\pm,\mathrm{DH}} = -\frac{A|z_+z_-|(I^{1/2})}{1 + B\mathring{a}(I^{1/2})} \qquad (3)$$

Table I. Osmotic Coefficients in Dilute Aqueous Calcium Chloride Solutions at 25 °C ($\mathring{a}$ = 4.65 × 10^{-8} cm, h = 12.3)

m	ϕ_{DH}	$0.018hm$	ϕ	
			Eq 9	Ref 3
0.0001	0.9864	0.00002	0.9864	0.9869
0.0005	0.9720	0.0001	0.9721	0.9719
0.001	0.9619	0.0002	0.9621	0.9615
0.002	0.9485	0.0004	0.9489	—
0.003	0.9392	0.0007	0.9399	—
0.004	0.9319	0.0009	0.9328	—
0.005	0.9258	0.0011	0.9269	0.9250
0.006	0.9205	0.0013	0.9218	—
0.007	0.9160	0.0015	0.9175	—
0.008	0.9118	0.0018	0.9136	—
0.009	0.9080	0.0020	0.9100	—
0.01	0.9046	0.0022	0.9068	0.9048
0.02	0.8812	0.0044	0.8856	0.884
0.003	0.8671	0.0066	0.8737	—
0.04	0.8572	0.0089	0.8661	0.867
0.05	0.8498	0.0111	0.8609	0.861
0.06	0.8441	0.0133	0.8574	—
0.07	0.8394	0.0155	0.8549	0.857
0.08	0.8356	0.0177	0.8533	—
0.09	0.8323	0.0199	0.8522	—
0.1	0.8295	0.0221	0.8516	0.854

where I is the ionic strength reckoned on a molar concentration scale, $\mathring{a}$ is the ion-size parameter, z_+ and z_- are charge numbers on the cation and the anion, respectively, and A and B are constants. For aqueous solutions at 25 °C, $A = 0.5115$ mol$^{-1/2}$ L$^{1/2}$, and $B = 0.3291 \times 10^8$ cm^{-1} mol$^{-1/2}$ L$^{1/2}$ (*5*).

In dilute single electrolyte solutions, the molar ionic strength in eq 3 may be expressed as follows (*4*)

$$I \approx \frac{1}{2}|z_+z_-|\nu d_0 m \tag{4}$$

in which d_0 is the density of water; at 25 °C, $d_0 = 0.997\,07$ g cm^{-3} (*5*).

Therefore, the Debye-Hückel equation can be written

$$\ln f_{\pm,\mathrm{DH}} = -\frac{\frac{\ln 10}{\sqrt{2}} A\nu^{1/2} d_0^{1/2}|z_+z_-|^{3/2} m^{1/2}}{1 + \frac{1}{\sqrt{2}} B\mathring{a}\nu^{1/2} d_0^{1/2}|z_+z_-|^{1/2} m^{1/2}} = \frac{k_1 m^{1/2}}{1 + K_2 m^{1/2}} \tag{5}$$

where

$$K_1 = -\frac{\ln 10}{\sqrt{2}} A\nu^{1/2} d_0^{1/2}|z_+z_-|^{3/2} \tag{6}$$

$$K_2 = \frac{1}{\sqrt{2}} B\mathring{a}\nu^{1/2} d_0^{1/2}|z_+z_-|^{1/2} \tag{7}$$

For 1–1 electrolytes, $K_1 = -1.176\,04$, $K_2 = 0.328\,618 \times 10^8\mathring{a}$; and for 2–1 electrolytes, $K_1 = -4.073\,93$, $K_2 = 0.569\,182 \times 10^8\mathring{a}$.

The molal osmotic coefficients of a solution are related to the mean molal activity coefficients of the electrolyte by means of the Gibbs–Duhem relation. One convenient form (*5*) is

$$\phi = 1 + \frac{1}{m}\int_0^m m\,d\ln\gamma_\pm \tag{8}$$

By substituting eq 2 and 5 into eq 8, we obtain

$$\phi = 1 + \frac{K_1}{K_2^3 m}\left[(1 + K_2 m^{1/2}) - 2\ln(1 + K_2 m^{1/2}) - (1 + K_2 m^{1/2})^{-1}\right] + 0.018(h - \nu/2)m \tag{9}$$

If the hydration effect is ignored ($h = 0$), then ϕ in eq 9 represents ϕ_{DH}, the osmotic coefficient of solution calculated from the Debye–Hückel equation, i.e.

$$\phi_{DH} = 1 + \frac{1}{m}\int_0^m m\,d\ln\gamma_{\pm,\mathrm{DH}} \tag{10}$$

where

$$\ln\gamma_{\pm,\mathrm{DH}} = \ln f_{\pm,\mathrm{DH}} - \ln(1 + 0.018\nu m) \approx \ln f_{\pm,\mathrm{DH}} - 0.018\nu m \tag{11}$$

Table II. Activity and Osmotic Coefficients in Dilute Aqueous Alkaline Earth Chloride Solutions at 25 °C [a]

m	Activity coefficient				Osmotic coefficient			
	$MgCl_2$	$CaCl_2$	$SrCl_2$	$BaCl_2$	$MgCl_2$	$CaCl_2$	$SrCl_2$	$BaCl_2$
0.0001	0.9612	0.9611	0.9611	0.9611	0.9865	0.9864	0.9867	0.9867
0.0005	0.9180	0.9178	0.9178	0.9177	0.9723	0.9721	0.9723	0.9722
0.001	0.8887	0.8883	0.8883	0.8882	0.9623	0.9621	0.9621	0.9621
0.002	0.8510	0.8503	0.8505	0.8502	0.9495	0.9489	0.9491	0.9490
0.003	0.8249	0.8239	0.8240	0.8237	0.9403	0.9399	0.9400	0.9398
0.004	0.8044	0.8032	0.8034	0.8029	0.9336	0.9328	0.9329	0.9326
0.005	0.7876	0.7861	0.7863	0.7857	0.9278	0.9269	0.9269	0.9266
0.006	0.7731	0.7714	0.7716	0.7710	0.9228	0.9218	0.9220	0.9216
0.007	0.7605	0.7586	0.7588	0.7580	0.9186	0.9175	0.9175	0.9170
0.008	0.7493	0.7471	0.7473	0.7465	0.9149	0.9136	0.9136	0.9130
0.009	0.7391	0.7368	0.7370	0.7361	0.9115	0.9100	0.9101	0.9095
0.01	0.7299	0.7274	0.7276	0.7266	0.9085	0.9068	0.9069	0.9063
0.02	0.6667	0.6627	0.6628	0.6610	0.8884	0.8856	0.8855	0.8841
0.03	0.6289	0.6237	0.6236	0.6216	0.8774	0.8737	0.8734	0.8714
0.04	0.6023	0.5962	0.5959	0.5926	0.8707	0.8661	0.8656	0.8628
0.05	0.5825	0.5753	0.5748	0.5709	0.8664	0.8609	0.8601	0.8567
0.06	0.5668	0.5587	0.5579	0.5533	0.8636	0.8574	0.8559	0.8520
0.07	0.5539	0.5451	0.5440	0.5388	0.8618	0.8549	0.8534	0.8486
0.08	0.5432	0.5337	0.5323	0.5265	0.8609	0.8533	0.8513	0.8458
0.09	0.5342	0.5240	0.5223	0.5159	0.8605	0.8522	0.8499	0.8437
0.1	0.5264	0.5156	0.5136	0.5066	0.8606	0.8516	0.8489	0.8421

[a] Values of $\mathring{a}$ (Å): $MgCl_2$ (4.83); $CaCl_2$ (4.65); $SrCl_2$ (4.74); $BaCl_2$ (4.74). Values of h: $MgCl_2$ (14.7); $CaCl_2$ (12.3); $SrCl_2$ (9.5); $BaCl_2$ (5.7).

Table III. Activity and Osmotic Coefficients in Dilute Aqueous Alkaline Earth Bromide Solutions at 25 °C

	Activity coefficient				Osmotic coefficient			
m	$MgBr_2$	$CaBr_2$	$SrBr_2$	$BaBr_2$	$MgBr_2$	$CaBr_2$	$SrBr_2$	$BaBr_2$
0.0001	0.9612	0.9612	0.9612	0.9611	0.9866	0.9866	0.9866	0.9867
0.0005	0.9182	0.9181	0.9180	0.9178	0.9724	0.9723	0.9723	0.9723
0.001	0.8890	0.8888	0.8887	0.8884	0.9625	0.9624	0.9624	0.9622
0.002	0.8517	0.8513	0.8512	0.8505	0.9498	0.9496	0.9495	0.9491
0.003	0.8258	0.8253	0.8251	0.8242	0.9410	0.9407	0.9406	0.9401
0.004	0.8056	0.8050	0.8047	0.8035	0.9341	0.9339	0.9337	0.9329
0.005	0.7889	0.7882	0.7879	0.7864	0.9286	0.9281	0.9279	0.9270
0.006	0.7747	0.7738	0.7735	0.7718	0.9238	0.9233	0.9230	0.9221
0.007	0.7623	0.7613	0.7609	0.7590	0.9197	0.9191	0.9188	0.9176
0.008	0.7512	0.7502	0.7497	0.7475	0.9161	0.9154	0.9150	0.9137
0.009	0.7413	0.7401	0.7396	0.7373	0.9129	0.9121	0.9117	0.9103
0.01	0.7323	0.7310	0.7304	0.7279	0.9099	0.9090	0.9086	0.9071
0.02	0.6708	0.6684	0.6673	0.6633	0.8912	0.8894	0.8886	0.8858
0.03	0.6344	0.6310	0.6294	0.6243	0.8815	0.8788	0.8776	0.8740
0.04	0.6093	0.6049	0.6029	0.5967	0.8761	0.8725	0.8708	0.8663
0.05	0.5905	0.5853	0.5828	0.5758	0.8725	0.8680	0.8660	0.8610
0.06	0.5760	0.5698	0.5669	0.5591	0.8712	0.8658	0.8633	0.8572
0.07	0.5642	0.5572	0.5540	0.5454	0.8705	0.8642	0.8613	0.8546
0.08	0.5546	0.5467	0.5431	0.5339	0.8707	0.8635	0.8602	0.8528
0.09	0.5467	0.5379	0.5339	0.5240	0.8714	0.8633	0.8596	0.8515
0.1	0.5399	0.5303	0.5259	0.5154	0.8725	0.8635	0.8593	0.8507

[a] Values of $\mathring{a}$ (Å): $MgBr_2$ (4.92); $CaBr_2$ (4.92); $SrBr_2$ (4.92); $BaBr_2$ (4.74). Values of h: $MgBr_2$ (20.1); $CaBr_2$ (15.1); $SrBr_2$ (12.8); $BaBr_2$ (10.5).

Table IV. Activity and Osmotic Coefficients in Dilute Aqueous Alkaline Earth Perchlorate Solutions at 25 °C

	Activity coefficient				Osmotic coefficient			
m	$Mg(ClO_4)_2$	$Ca(ClO_4)_2$	$Sr(ClO_4)_2$	$Ba(ClO_4)_2$	$Mg(ClO_4)_2$	$Ca(ClO_4)_2$	$Sr(ClO_4)_2$	$Ba(ClO_4)_2$
0.0001	0.9614	0.9613	0.9612	0.9612	0.9870	0.9868	0.9867	0.9866
0.0005	0.9189	0.9185	0.9180	0.9180	0.9728	0.9726	0.9724	0.9723
0.001	0.8905	0.8896	0.8886	0.8887	0.9633	0.9628	0.9623	0.9624
0.002	0.8584	0.8527	0.8510	0.8512	0.9513	0.9504	0.9494	0.9495
0.003	0.8294	0.8272	0.8248	0.8250	0.9431	0.9418	0.9405	0.9406
0.004	0.8102	0.8074	0.8044	0.8046	0.9369	0.9353	0.9335	0.9337
0.005	0.7944	0.7911	0.7875	0.7878	0.9318	0.9299	0.9277	0.9278
0.006	0.7809	0.7772	0.7731	0.7733	0.9276	0.9253	0.9229	0.9229
0.007	0.7693	0.7651	0.7605	0.7607	0.9240	0.9214	0.9187	0.9187
0.008	0.7589	0.7543	0.7493	0.7495	0.9208	0.9180	0.9149	0.9149
0.009	0.7497	0.7446	0.7392	0.7394	0.9180	0.9150	0.9116	0.9116
0.01	0.7413	0.7359	0.7300	0.7302	0.9155	0.9122	0.9086	0.9085
0.02	0.6849	0.6763	0.6672	0.6669	0.9004	0.8947	0.8888	0.8883
0.03	0.6524	0.6413	0.6297	0.6289	0.8936	0.8861	0.8783	0.8772
0.04	0.6305	0.6173	0.6037	0.6022	0.8905	0.8814	0.8721	0.8703
0.05	0.6145	0.5995	0.5843	0.5820	0.8895	0.8790	0.8683	0.8653
0.06	0.6024	0.5857	0.5690	0.5660	0.8897	0.8779	0.8660	0.8624
0.07	0.5930	0.5748	0.5566	0.5528	0.8909	0.8778	0.8648	0.8603
0.08	0.5855	0.5658	0.5465	0.5419	0.8927	0.8784	0.8644	0.8590
0.09	0.5796	0.5584	0.5379	0.5325	0.8949	0.8795	0.8646	0.8583
0.1	0.5748	0.5523	0.5307	0.5244	0.8975	0.8810	0.8653	0.8579

[a] Values of $\mathring{a}$ (Å): $Mg(ClO_4)_2$ (5.70); $Ca(ClO_4)_2$ (5.26); $Sr(ClO_4)_2$ (5.74); $Ba(ClO_4)_2$ (4.92). Values of h: $Mg(ClO_4)_2$ (24.3); $Ca(ClO_4)_2$ (20.4); $Sr(ClO_4)_2$ (18.6); $Ba(ClO_4)_2$ (12.0).

Thus Equation 9 becomes

$$\phi_{DH} = 1 + \frac{K_1}{K_2{}^3 m}[(1 + K_2 m)^{1/2}) - 2 \ln (1 + K_2 m^{1/2}) - (1 + K_2 m^{1/2})^{-1}] - 0.009\nu m \qquad (12)$$

Therefore, the modification term due to hydration is $0.018hm$. Equation 9 takes the form

$$\phi = \phi_{DH} + 0.018hm \qquad (13)$$

The last term on the right side of eq 12 is derived from the relationship between the mean rational activity coefficient and the mean molal activity coefficient (*5*). In a very dilute solution, this term may be ignored.

Activity and osmotic coefficients in dilute aqueous electrolyte solutions thus can be obtained from eq 1 and 9 if suitable values of $\mathring{a}$ and h are available. Guggenheim and Stokes (*1*) have compiled the revised values of $\mathring{a}$ and h for some 1–1 electrolytes as well as 2–1 electrolytes. Their data are somewhat different from the data that appeared in Stokes and Robinson's original article (*6*), or the data compiled in Robinson and Stokes' book (*5*). The activity and osmotic coefficients in some 2–1 electrolyte solutions are calculated by use of Guggenheim and Stokes' data. Table I shows the hydration effects on the osmotic coefficients in calcium chloride solutions, and also the validity of the derived equations. The calculated values of osmotic coefficients in these solutions agree satisfactorily with the data compiled by Pitzer and Brewer (*3*) in the concentration range up to 0.1 m. Activity and osmotic coefficients in dilute solutions of some 2–1 electrolytes, including chlorides, bromides, and perchlorates, are calculated and compiled in Tables II, III, and IV. The maximum estimated error for these values is about 0.3%.

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NEW COMPOUND SECTION

The Synthesis of Derivatives of 3,7-Diazanonanedioic Acid

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The synthesis of several esters of 2,8-disubstituted 3,7-diazanonanedioic acid from amino acid esters and 1,3-dibromopropane is described. The compounds reported include ethyl 3,7-diaza-2,8-di(isobutyl)nonanedioate, methyl 3,7-diaza-2,8-(3-thiabutyl)nonanedioate, ethyl 3,7-diaza-2,8-dimethylnonanedioate, ethyl 3,7-diaza-2,8-dibenzylnonanedioate, and benzyl 3,7-diaza-2,8-dimethylnonanedioate.

As part of a study of multidentate ligands, it was desired to prepare symmetrical amino esters of the general formula $(XO_2CCHRNHCH_2)_2CH_2$ (I), where R could be the side chain groups of the naturally occurring amino acids. We wish to report the synthesis of several of these esters of 2,8-disubstituted 3,7-diazanonanedioic acid by a simple, direct route (*1*).

A mixture of two parts amino acid ester hydrochloride, one part 1,3-dibromopropane, and four parts triethylamine was heated for several days in a suitable solvent. The product was isolated by extraction and purified by chromatography. The structures of the resulting di(amino esters) (Table I) were confirmed by spectral data and analysis of the dihydrochloride derivatives.

$$BrCH_2CH_2CH_2Br + 2NH_2CHRCO_2X \xrightarrow{Et_3N} XO_2CCHRNHCH_2CH_2CH_2NHCHRCO_2X$$

When exposed to the atmosphere, these compounds are stable for several days. After this time a precipitate slowly forms in the oils. Infrared analysis of this precipitate shows amine salt and carboxylate peaks, indicating that it is a hydrolysis product.

Table I. Derivatives of 3,7-Diazanonanedioic Acid $XO_2CCHRNHCH_2CH_2CH_2NHCHRCO_2X$

Compound	R	X	Solvent	Yield (%)	Mp of dihydrochloride (°C)
1a	H–	Et–	EtOH	23	——[a]
b	$(CH_3)_2CHCH_2$–	Et–	EtOH	51	178–180
c	$CH_3SCH_2CH_2$–	Me–	MeOH	35	158–160
d	CH_3–	Et–	EtOH	56	151–153
e	$C_6H_5CH_2$–	Et–	EtOH	50	168–169
f	CH_3–	$C_6H_5CH_2$–	Dioxane	29	243–245

[a] An analytically pure sample of this compound could not be obtained.

Table II. IR Data for Compounds Ia–f

Compound	IR data (thin film), cm^{-1} N—H	C=O	C—O	Other absorptions
Ia	3400	1748	1170	950, 910, 755
b	3380	1730	1170	935, 860, 755
c	3390	1736	1050	990, 915, 900, 760-750
d	3356	1727	1170	1030, 860, 755
e	3352	1730	1170	1090, 755, 700
f	3390	1730	1170	740, 695