Molar Volumes and Refractive Indexes of Hexane-1,2,3,4,5,6-hexol in Aqueous Solutions of 1-Propanol and 2-Propanol

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Apparent molar volumes (V_Φ) of hexane-1,2,3,4,5,6-hexol in aqueous solutions of 1- and 2-propanols were obtained from densities of ternary solutions, accurately measured with a quartz vibrating-tube densimeter at several temperatures in the range from (293.15 to 313.15) K. Refractive indexes (n_D) measurements were also made for hexane-1,2,3,4,5,6-hexol + propanol + water at $T = 298.15$ K. The data of V_Φ have been used to deduce the limiting partial molar volumes of hexane-1,2,3,4,5,6-hexol (V^0_Φ) and limiting partial molar volumes of transfer ($\Delta_{trs}V^0_\Phi$) from water to different alcohol solutions at different concentrations. From the values of n_D, molar refractive indexes (R_D) were calculated. Then the changes of these parameters were discussed in the light of interaction between solute and solvent and the different locations of the hydroxyl group in propanol isomers.

Introduction

Intermolecular interactions have been largely investigated in the last few decades through thermodynamic methods such as those based on density and the refractive index.[1−6] Volumetric properties of solute in an aqueous system, such as partial molar volume, are known to be sensitive to the degree and nature of solute hydration. The partial molar volume of a solute includes the structural volume of the solute in the solvent and the volume change of the solvent in the process of solvation shell formation around the solute particles.[7] At low solute concentrations, the measured volume reflects the contribution of both solvent effect and solute intrinsic properties.[8]

Hexane-1,2,3,4,5,6-hexol is a naturally occurring six-carbon sugar alcohol (polyol),[9] which is widely used in many fields of medicine because of its beneficial action on the brain,[10−14] kidneys,[15] and heart of humans.[16] In addition, the hydration characteristics of saccharides in aqueous solutions are a key feature in determining their structural and functional properties.[17] Aqueous solutions of alcohols have served as useful industrial solvent media for a variety of separation processes and pharmaceutical applications and also become more popular to use in solar thermal systems.[18] In a word, it is of significance to study the interactions of hexane-1,2,3,4,5,6-hexol with propanol in an aqueous system. However, to our knowledge, there has been no report on the density values of hexane-1,2,3,4,5,6-hexol in aqueous alcohol solutions. In this paper, we present densities (ρ), apparent molar volumes (V_Φ), limiting partial molar volumes (V^0_Φ), and transfer partial molar volumes ($\Delta_{trs}V^0_\Phi$) from water to different alcohol solutions at different temperatures. For a better understanding of the weak interactions of the solute with the solvent, refractive indexes were measured, and corresponding molar refractive indexes (at 298.15 K) were acquired and considered.

Experimental Section

Materials. Hexane-1,2,3,4,5,6-hexol was a product of Aldrich company, and the stated mass fraction purity was better than 0.99. 1-Propanol and 2-propanol were all analytical reagents, purchased from Shanghai Chemical Reagent Company (Shanghai, China) and refined by vacuum distillation before use (mass fraction purity ≥ 0.997). Twice-distilled water was used in the experiment. Solutions of different compositions were prepared by weight using a Mettler Toledo AG 135 analytical balance with a precision of $\pm 1 \cdot 10^{-5}$ g.

Density Measurement. The densities of solutions were measured by a quartz vibrating-tube densimeter (Anton Paar DMA 5000) thermostated to better than ± 0.001 K. The precision of the densimeter was $\pm 2 \cdot 10^{-6}$ g·cm^{-3}, which was nearly the same as that of the Anton Paar DSA 5000 vibrating-tube digital densimeter.[19,20] This instrument was calibrated with twice-distilled water and dried air. The densities of twice-distilled water we measured were 0.998205 g·cm^{-3} and 0.997045 g·cm^{-3} at $T = 293.15$ K and $T = 298.15$ K, respectively, which were within the experimental uncertainty of the literature values.[21,22] The average of triplicate measurements for each sample was as its final result, and all of the density data are gathered in Table 1.

Refractive Index Measurement. Refractive indexes were measured on a model-2W refractometer (Shanghai, China), which was calibrated with pure water whose measured refractive index at 298.15 K was 1.3326 ± 0.0003 (mean value of five iterations). This value agreed well with that in literature.[23] The data of refractive indexes are also listed in Table 1.

Results and Discussion

Change Tendency of Density in the Ternary System. The data in Table 1 show that in the experimental ranges of concentration and temperature, the density of solution becomes larger with the increase of hexane-1,2,3,4,5,6-hexol concentration whether in pure water or in the water−propanol solvent mixture. This phenomenon means that hexane-1,2,3,4,5,6-hexol molecules can shorten the mean distance between molecules in the solution, which might be explained by considering the strong polarity and hydrophility of the polyol.

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Table 1. Densities (ρ), Refractive Indexes (n_D), and Molar Refractive Indexes (R_D) of the Solutions and Apparent Molar Volumes (V_Φ) of Hexane-1,2,3,4,5,6-hexol in Water and Aqueous Solutions of 1- and 2-Propanols

$m_{\text{hexane-1,2,3,4,5,6-hexol}}$	ρ	V_Φ	ρ	V_Φ	ρ	V_Φ	ρ	V_Φ	ρ	V_Φ		$10^{-12}\cdot R_D$
mol·kg^{-1}	g·cm^{-3}	cm^3·mol^{-1}	g·cm^{-3}	cm^3·mol^{-1}	g·cm^{-3}	cm^3·mol^{-1}	g·cm^{-3}	cm^3·mol^{-1}	g·cm^{-3}	cm^3·mol^{-1}	n_D	cm^3·mol^{-1}
	293.15 K		298.15 K		303.15 K		308.15 K		313.15 K		298.15 K	
					H_2O							
0.0000	0.998205		0.997045		0.995645		0.994027		0.992212		1.3326	3.7094
0.1000	1.004395	119.61	1.003213	119.90	1.001786	120.26	1.000125	120.79	0.998283	121.17	1.3358	3.7823
0.1499	1.007499	119.18	1.006298	119.53	1.004865	119.83	1.003190	120.32	1.001328	120.74	1.3370	3.8116
0.1999	1.010610	118.76	1.009401	119.07	1.007949	119.42	1.006229	120.03	1.004362	120.40	1.3385	3.8459
0.2500	1.013687	118.52	1.012458	118.86	1.010982	119.25	1.009258	119.78	1.007369	120.18	1.3396	3.8763
0.3000	1.016747	118.27	1.015475	118.72	1.013991	119.08	1.012248	119.60	1.010330	120.06	1.3410	3.9097
0.3500	1.019738	118.20	1.018461	118.61	1.016974	118.95	1.015194	119.52	1.013262	119.97	1.3422	3.9412
0.4000	1.022709	118.11	1.021426	118.49	1.019919	118.85	1.018126	119.39	1.016177	119.84	1.3430	3.9685
					$m_{1\text{-propanol}} = 0.1001$ mol·kg^{-1}							
0.0000	0.996609		0.995441		0.994029		0.992397		0.990564		1.3331	3.7362
0.1000	1.002706	120.30	1.001520	120.55	1.000083	120.89	0.998407	121.44	0.996536	121.94	1.3360	3.8049
0.1500	1.005814	119.53	1.004611	119.84	1.003167	120.14	1.001477	120.63	0.999577	121.20	1.3372	3.8363
0.2000	1.008905	119.06	1.007701	119.31	1.006238	119.65	1.004505	120.26	1.002620	120.64	1.3385	3.8688
0.2500	1.011965	118.74	1.010734	119.07	1.009256	119.42	1.007514	119.97	1.005605	120.39	1.3398	3.9013
0.3000	1.015022	118.44	1.013742	118.89	1.012242	119.27	1.010471	119.84	1.008556	120.23	1.3410	3.9330
0.3501	1.018005	118.35	1.016720	118.76	1.015181	119.22	1.013422	119.69	1.011479	120.12	1.3421	3.9636
0.4000	1.020968	118.23	1.019662	118.65	1.018099	119.12	1.016325	119.58	1.014362	120.03	1.3435	3.9974
					$m_{1\text{-propanol}} = 0.1500$ mol·kg^{-1}							
0.0000	0.996479		0.995293		0.993828		0.992237		0.990399		1.3338	3.7515
0.1000	1.002478	120.43	1.001299	120.62	0.999852	121.03	0.998174	121.58	0.996305	122.04	1.3363	3.8168
0.1501	1.005592	119.56	1.004389	119.87	1.002932	120.24	1.001242	120.72	0.999349	121.23	1.3376	3.8494
0.1999	1.008663	119.08	1.007460	119.33	1.005995	119.67	1.004260	120.29	1.002372	120.67	1.3388	3.8809
0.2499	1.011718	118.76	1.010488	119.08	1.009006	119.44	1.007263	119.99	1.005350	120.42	1.3401	3.9136
0.3000	1.014769	118.46	1.013458	119.02	1.011982	119.31	1.010211	119.88	1.008297	120.26	1.3415	3.9476
0.3501	1.017741	118.38	1.016441	118.83	1.014921	119.23	1.013152	119.72	1.011211	120.15	1.3426	3.9783
0.4000	1.020661	118.32	1.019361	118.73	1.017819	119.14	1.016036	119.62	1.014099	119.99	1.3439	4.0111
					$m_{1\text{-propanol}} = 0.2000$ mol·kg^{-1}							
0.0000	0.996336		0.995163		0.993747		0.992113		0.990278		1.3341	3.7630
0.1001	1.002377	120.58	1.001187	120.83	0.999743	121.20	0.998071	121.69	0.996199	122.18	1.3366	3.8285
0.1500	1.005471	119.65	1.004263	119.96	1.002804	120.34	1.001125	120.74	0.999231	121.26	1.3375	3.8570
0.1999	1.008549	119.11	1.007341	119.35	1.005873	119.70	1.004140	120.31	1.002252	120.70	1.3388	3.8896
0.2500	1.011599	118.78	1.010365	119.10	1.008881	119.46	1.007132	120.04	1.005215	120.48	1.3400	3.9213
0.3001	1.014638	118.48	1.013355	118.93	1.011848	119.33	1.010072	119.91	1.008159	120.29	1.3411	3.9521
0.3499	1.017591	118.39	1.016298	118.82	1.014769	119.23	1.012981	119.79	1.011040	120.21	1.3426	3.9871
0.4001	1.020532	118.31	1.019222	118.73	1.01768	119.14	1.015885	119.66	1.013925	120.09	1.3437	4.0181
					$m_{1\text{-propanol}} = 0.3000$ mol·kg^{-1}							
0.0000	0.995903		0.994694		0.993242		0.991569		0.989694		1.3344	3.7835
0.1000	1.001858	121.09	1.000609	121.57	0.999129	121.95	0.997408	122.55	0.995513	122.88	1.3369	3.8501
0.1501	1.004911	120.23	1.003660	120.59	1.002169	120.94	1.000432	121.49	0.998514	121.90	1.3381	3.8820
0.2000	1.007973	119.54	1.006676	120.07	1.005168	120.44	1.003408	121.00	1.001503	121.27	1.3393	3.9140
0.2500	1.010998	119.14	1.009699	119.59	1.008172	119.99	1.006399	120.50	1.004471	120.84	1.3405	3.9459
0.3000	1.013949	119.03	1.012629	119.48	1.011096	119.85	1.009333	120.26	1.007362	120.71	1.3418	3.9791
0.3500	1.016870	118.93	1.015587	119.22	1.013995	119.73	1.012205	120.18	1.010248	120.53	1.3432	4.0133
0.4000	1.019766	118.84	1.018478	119.12	1.016868	119.61	1.015059	120.07	1.013089	120.43	1.3444	4.0455
					$m_{1\text{-propanol}} = 0.4000$ mol·kg^{-1}							
0.0000	0.994270		0.993072		0.991629		0.989962		0.988093		1.3349	3.8104
0.1001	1.000183	121.28	0.998943	121.79	0.997470	122.19	0.995765	122.69	0.993864	123.15	1.3378	3.8824
0.1499	1.003222	120.29	1.001969	120.74	1.000483	121.13	0.998766	121.58	0.996838	122.11	1.3388	3.9124
0.2000	1.006274	119.60	1.005008	120.03	1.003486	120.53	1.001741	121.04	0.999844	121.30	1.3400	3.9446
0.2501	1.009255	119.35	1.008007	119.63	1.006446	120.21	1.004687	120.69	1.002759	121.06	1.3411	3.9757
0.3000	1.012182	119.22	1.010923	119.50	1.009337	120.09	1.007592	120.46	1.005642	120.86	1.3422	4.0071
0.3500	1.015098	119.08	1.013819	119.39	1.012231	119.92	1.010437	120.40	1.008524	120.64	1.3440	4.0459
0.4000	1.017962	119.03	1.016665	119.36	1.015078	119.82	1.013304	120.21	1.011346	120.55	1.3450	4.0764
					$m_{1\text{-propanol}} = 0.5000$ mol·kg^{-1}							
0.0000	0.993364		0.992148		0.990687		0.989004		0.987114		1.3353	3.8337
0.0999	0.999212	121.58	0.997964	121.99	0.996468	122.45	0.994743	123.00	0.992826	123.41	1.3380	3.9050
0.1501	1.002261	120.42	1.001001	120.80	0.999489	121.24	0.997757	121.69	0.995809	122.22	1.3391	3.9363
0.2000	1.005268	119.83	1.004002	120.16	1.002451	120.72	1.000699	121.19	0.998785	121.43	1.3403	3.9687
0.2500	1.008225	119.54	1.006960	119.82	1.005383	120.40	1.003609	120.89	1.001664	121.23	1.3414	4.0001
0.3000	1.011131	119.42	1.009860	119.68	1.008271	120.22	1.006505	120.62	1.004540	121.00	1.3426	4.0327
0.3500	1.014019	119.31	1.012737	119.58	1.011134	120.10	1.009352	120.50	1.007393	120.82	1.3442	4.0697
0.4000	1.016881	119.20	1.015604	119.43	1.014037	119.80	1.012202	120.30	1.010224	120.65	1.3454	4.1024
					$m_{2\text{-propanol}} = 0.1000$ mol·kg^{-1}							
0.0000	0.996544		0.995386		0.993986		0.992365		0.990542		1.3329	3.7343
0.1000	1.002684	119.84	1.001499	120.19	1.000069	120.58	0.998398	121.18	0.996541	121.64	1.3360	3.8049
0.1500	1.005789	119.26	1.004578	119.68	1.003135	120.06	1.001452	120.58	0.999562	121.15	1.3371	3.8354
0.2000	1.008882	118.85	1.007675	119.16	1.006209	119.58	1.004485	120.21	1.002605	120.61	1.3385	3.8688
0.2500	1.011950	118.54	1.010701	118.98	1.009221	119.39	1.007495	119.92	1.005594	120.35	1.3398	3.9014
0.3000	1.014995	118.31	1.013717	118.79	1.012206	119.25	1.010470	119.74	1.008542	120.21	1.3410	3.9330
0.3500	1.017983	118.22	1.016685	118.69	1.015146	119.19	1.013408	119.63	1.011462	120.10	1.3421	3.9637
0.4000	1.020946	118.12	1.019629	118.59	1.018065	119.10	1.016315	119.53	1.014365	119.97	1.3434	3.9965
					$m_{2\text{-propanol}} = 0.1501$ mol·kg^{-1}							
0.0000	0.995924		0.994764		0.993358		0.991731		0.989901		1.3335	3.7506
0.1001	1.002038	120.02	1.000854	120.33	0.999418	120.72	0.997744	121.30	0.995879	121.78	1.3362	3.8175
0.1499	1.005131	119.35	1.003918	119.78	1.002471	120.14	1.000787	120.63	0.998893	121.18	1.3372	3.8470
0.2000	1.008217	118.93	1.007009	119.24	1.005543	119.63	1.003812	120.26	1.001926	120.66	1.3388	3.8827

Table 1. Continued

$m_{\text{hexane-1,2,3,4,5,6-hexol}}$	ρ	V_Φ	ρ	V_Φ	ρ	V_Φ	ρ	V_Φ	ρ	V_Φ		$10^{-12}\cdot R_D$
mol·kg^{-1}	g·cm^{-3}	cm^3·mol^{-1}	g·cm^{-3}	cm^3·mol^{-1}	g·cm^{-3}	cm^3·mol^{-1}	g·cm^{-3}	cm^3·mol^{-1}	g·cm^{-3}	cm^3·mol^{-1}	n_D	cm^3·mol^{-1}
0.2500	1.011270	118.64	1.010028	119.04	1.008551	119.41	1.006816	119.96	1.004908	120.39	1.3401	3.9154
0.3000	1.014307	118.40	1.013019	118.90	1.011525	119.29	1.009770	119.82	1.007851	120.24	1.3413	3.9472
0.3500	1.017301	118.24	1.015986	118.77	1.014458	119.21	1.012699	119.69	1.010758	120.13	1.3426	3.9800
0.4000	1.020246	118.18	1.018921	118.67	1.017378	119.11	1.015599	119.60	1.013662	119.99	1.3439	4.0130
					$m_{2\text{-propanol}} = 0.1999$ mol·kg^{-1}							
0.0000	0.995400		0.994220		0.992795		0.991148		0.989299		1.3338	3.7636
0.1000	1.001474	120.24	1.000269	120.56	0.998815	120.94	0.997129	121.45	0.995242	121.95	1.3363	3.8289
0.1500	1.004576	119.44	1.003341	119.89	1.001872	120.28	1.000175	120.72	0.998265	121.25	1.3374	3.8596
0.2000	1.007644	119.02	1.006415	119.34	1.004938	119.69	1.003191	120.30	1.001289	120.69	1.3390	3.8953
0.2500	1.010681	118.76	1.009440	119.08	1.007943	119.46	1.006186	120.01	1.004251	120.48	1.3403	3.9281
0.3000	1.013722	118.46	1.012427	118.92	1.010914	119.31	1.009128	119.89	1.007204	120.26	1.3412	3.9568
0.3500	1.016700	118.32	1.015379	118.81	1.013842	119.22	1.012044	119.77	1.010099	120.16	1.3424	3.9887
0.4001	1.019639	118.25	1.018308	118.71	1.016757	119.12	1.014961	119.60	1.013003	120.00	1.3441	4.0260
					$m_{2\text{-propanol}} = 0.3000$ mol·kg^{-1}							
0.0000	0.994591		0.993429		0.992018		0.990384		0.988545		1.3341	3.7853
0.0999	1.000566	120.85	0.999334	121.29	0.997888	121.74	0.996228	122.11	0.994343	122.71	1.3368	3.8536
0.1499	1.003670	120.12	1.002411	120.49	1.000960	120.85	0.999274	121.31	0.997380	121.81	1.3385	3.8910
0.2000	1.006761	119.44	1.005454	119.89	1.003989	120.26	1.002304	120.62	1.000386	121.14	1.3392	3.9177
0.2500	1.009830	118.97	1.008483	119.44	1.007030	119.70	1.005313	120.14	1.003349	120.77	1.3405	3.9506
0.3000	1.012828	118.78	1.011451	119.24	1.010005	119.44	1.008259	119.93	1.006315	120.40	1.3416	3.9817
0.3500	1.015808	118.62	1.014398	119.07	1.012931	119.32	1.011162	119.82	1.009218	120.24	1.3429	4.0149
0.4000	1.018763	118.46	1.017325	118.89	1.015853	119.14	1.014081	119.60	1.012090	120.11	1.3443	4.0491
					$m_{2\text{-propanol}} = 0.3998$ mol·kg^{-1}							
0.0000	0.993922		0.992857		0.991441		0.989702		0.987816		1.3345	3.8070
0.1000	1.000013	121.05	0.998811	121.51	0.997360	121.96	0.995680	122.48	0.993813	122.82	1.3370	3.8746
0.1500	1.003055	120.19	1.001843	120.59	1.000387	120.95	0.998685	121.49	0.996799	121.88	1.3388	3.9131
0.2000	1.006107	119.50	1.004863	119.98	1.003388	120.37	1.001680	120.83	0.999788	121.18	1.3396	3.9410
0.2501	1.009098	119.23	1.007875	119.54	1.006411	119.81	1.004656	120.40	1.002729	120.86	1.3408	3.9732
0.3000	1.012060	119.00	1.010804	119.39	1.009336	119.65	1.007576	120.18	1.005625	120.66	1.3419	4.0044
0.3500	1.015001	118.82	1.013723	119.23	1.012232	119.54	1.010481	119.97	1.008496	120.51	1.3431	4.0368
0.4000	1.017893	118.72	1.016604	119.11	1.015105	119.42	1.013317	119.91	1.011331	120.39	1.3445	4.0714
					$m_{2\text{-propanol}} = 0.5000$ mol·kg^{-1}							
0.0000	0.993065		0.991893		0.990472		0.988826		0.986979		1.3350	3.8317
0.0999	0.998935	121.38	0.997738	121.71	0.996279	122.20	0.994587	122.79	0.992719	123.12	1.3375	3.9007
0.1500	1.001971	120.34	1.000760	120.68	0.999285	121.14	0.997581	121.65	0.995687	122.10	1.3390	3.9362
0.2000	1.004994	119.71	1.003778	120.01	1.002261	120.60	1.000538	121.11	0.998668	121.34	1.3401	3.9675
0.2500	1.007990	119.30	1.006726	119.76	1.005182	120.37	1.003460	120.79	1.001562	121.11	1.3412	3.9990
0.3000	1.010913	119.15	1.009635	119.60	1.008069	120.19	1.006357	120.53	1.004436	120.90	1.3424	4.0316
0.3500	1.013803	119.07	1.012537	119.43	1.010960	119.98	1.009203	120.42	1.007275	120.78	1.3435	4.0631
0.4000	1.016683	118.95	1.015403	119.30	1.013831	119.79	1.012042	120.27	1.010111	120.60	1.3448	4.0969

Apparent Molar Volume. Apparent molar volumes (V_Φ) of hexane-1,2,3,4,5,6-hexol in pure water were calculated from the density values using eq 1:[24]

$$V_\Phi = M_b/\rho - 1000(\rho - \rho^0)/(m_b\rho\rho^0) \quad (1)$$

where M_b is the molar mass of the solute (hexane-1,2,3,4,5,6-hexol), m_b is the molality of hexane-1,2,3,4,5,6-hexol in binary solution, and ρ^0 and ρ are the densities of the pure water and the solution, respectively.

In hexane-1,2,3,4,5,6-hexol + propanol + water, the apparent molar volumes of hexane-1,2,3,4,5,6-hexol (V_Φ) can be calculated by using

$$V_\Phi = M_b/\rho - (1000 + M_a m_a)(\rho - \rho^{0\prime})/(m_b\rho\rho^{0\prime}) \quad (2)$$

where m_a and m_b are the molalities for propanol and hexane-1,2,3,4,5,6-hexol in aqueous solutions, ρ is the density of the ternary aqueous solution, and $\rho^{0\prime}$ is the density of water + propanol, which can be regarded as solvent of hexane-1,2,3,4,5,6-hexol. The calculated values of V_Φ are also listed in Table 1. It can be observed from the values that V_Φ becomes smaller as hexane-1,2,3,4,5,6-hexol concentration increases. This fact might be explained by considering (i) the change in mean distance between each pair of the solute molecules and (ii) the solvent molecules draining away from the shells of the solute molecules.[25]

Limiting Partial Molar Volume and Transfer Partial Molar Volume. To investigate the solvent effect on the volumetric property of hexane-1,2,3,4,5,6-hexol and exclude the interaction between the solute molecules, the apparent molar volumes of hexane-1,2,3,4,5,6-hexol in infinite dilution solutions (limiting partial molar volumes, V^0_Φ) should be applied. When the molality of hexane-1,2,3,4,5,6-hexol is in a very dilute range, the following formula can be set up, and V^0_Φ can be obtained from the curve of V_Φ versus m_b by extrapolation.[26]

$$V_\Phi = V^0_\Phi + S_v m_b \quad (3)$$

where S_v is the slope of the straight line of V_Φ to m_b. The corresponding transfer partial molar volume of hexane-1,2,3,4,5,6-hexol from pure water to aqueous propanol solution, $\Delta_{trs}V^0_\Phi$, can be calculated as defined by eq 4

$$\Delta_{trs}V^0_\Phi = V^0_\Phi(\text{in aqueous propanol solution}) - V^0_\Phi(\text{in water}) \quad (4)$$

The data of limiting partial molar volumes and the transfer partial molar volumes of hexane-1,2,3,4,5,6-hexol in infinite dilution solutions are calculated and summarized in Table 2. The data in Table 2 clearly indicate that both V^0_Φ and $\Delta_{trs}V^0_\Phi$ become larger with the increase of propanol molality in the solvent mixture. The variation tendency can be shown more clearly by the curves in Figure 1 and explained by using the cosphere overlap model.[27,28] Furthermore, it is observed from Table 2 that the values of $\Delta_{trs}V^0_\Phi$ in the 1-propanol−water solvent mixture is larger than that in the 2-propanol−water solvent mixture. This fact might be explained as follows: the hydroxyl group of 2-propanol is located in the middle of the two methyl groups, so the interaction of hydroxyl groups between 2-propanol and hexane-1,2,3,4,5,6-hexol is im-

Table 2. Limiting Partial Molar Volumes (V^0_Φ) of Hexane-1,2,3,4,5,6-hexol in Different Solvents and Transfer Partial Molar Volumes ($\Delta_{trs}V^0_\Phi$) of Hexane-1,2,3,4,5,6-hexol from Water to Aqueous Solutions of Propanols at Different Temperatures

$m_{propanol}$	V^0_Φ	$\Delta_{trs}V^0_\Phi$	V^0_Φ	$\Delta_{trs}V^0_\Phi$	V^0_Φ	$\Delta_{trs}V^0_\Phi$	V^0_Φ	$\Delta_{trs}V^0_\Phi$	V^0_Φ	$\Delta_{trs}V^0_\Phi$
$mol \cdot kg^{-1}$	$cm^3 \cdot mol^{-1}$	$cm^3 \cdot mol^{-1}$	$cm^3 \cdot mol^{-1}$	$cm^3 \cdot mol^{-1}$	$cm^3 \cdot mol^{-1}$	$cm^3 \cdot mol^{-1}$	$cm^3 \cdot mol^{-1}$	$cm^3 \cdot mol^{-1}$	$cm^3 \cdot mol^{-1}$	$cm^3 \cdot mol^{-1}$
	293.15 K		298.15 K		303.15 K		308.15 K		313.15 K	
					H_2O					
0.0000	120.85 ± 0.12	0.00	121.30 ± 0.20	0.00	121.73 ± 0.18	0.00	122.17 ± 0.09	0.00	122.65 ± 0.26	0.00
					1-Propanol					
0.1001	122.58 ± 0.06	1.73 ± 0.06	123.09 ± 0.05	1.79 ± 0.15	123.60 ± 0.11	1.87 ± 0.07	124.08 ± 0.16	1.91 ± 0.07	124.63 ± 0.13	1.98 ± 0.13
0.1500	122.96 ± 0.05	2.11 ± 0.07	123.48 ± 0.10	2.18 ± 0.10	123.99 ± 0.08	2.26 ± 0.10	124.51 ± 0.12	2.34 ± 0.03	125.05 ± 0.06	2.40 ± 0.20
0.2002	123.40 ± 0.06	2.55 ± 0.06	123.95 ± 0.13	2.65 ± 0.07	124.47 ± 0.18	2.75 ± 0.00	124.98 ± 0.16	2.81 ± 0.07	125.53 ± 0.22	2.88 ± 0.04
0.3001	124.22 ± 0.14	3.37 ± 0.02	124.72 ± 0.08	3.42 ± 0.12	125.20 ± 0.06	3.47 ± 0.12	125.70 ± 0.12	3.53 ± 0.03	126.23 ± 0.10	3.58 ± 0.16
0.4000	124.97 ± 0.05	4.12 ± 0.07	125.50 ± 0.05	4.20 ± 0.15	125.98 ± 0.10	4.25 ± 0.08	126.50 ± 0.08	4.33 ± 0.01	127.06 ± 0.11	4.41 ± 0.15
0.5000	125.80 ± 0.08	4.95 ± 0.04	126.33 ± 0.06	5.03 ± 0.14	126.84 ± 0.06	5.11 ± 0.12	127.36 ± 0.12	5.19 ± 0.03	127.91 ± 0.14	5.26 ± 0.12
					2-Propanol					
0.1000	121.54 ± 0.05	0.69 ± 0.07	122.03 ± 0.10	0.74 ± 0.10	122.51 ± 0.13	0.78 ± 0.05	123.03 ± 0.07	0.86 ± 0.02	123.55 ± 0.06	0.90 ± 0.20
0.1501	121.93 ± 0.22	1.08 ± 0.10	122.45 ± 0.13	1.15 ± 0.07	122.94 ± 0.09	1.21 ± 0.09	123.45 ± 0.08	1.28 ± 0.01	123.98 ± 0.16	1.33 ± 0.10
0.1999	122.49 ± 0.15	1.64 ± 0.03	122.99 ± 0.11	1.69 ± 0.09	123.50 ± 0.20	1.77 ± 0.02	124.00 ± 0.14	1.83 ± 0.05	124.54 ± 0.24	1.89 ± 0.02
0.3000	123.31 ± 0.22	2.46 ± 0.10	123.84 ± 0.19	2.54 ± 0.01	124.35 ± 0.28	2.62 ± 0.10	124.86 ± 0.10	2.69 ± 0.01	125.39 ± 0.06	2.74 ± 0.20
0.3998	124.10 ± 0.17	3.25 ± 0.05	124.60 ± 0.24	3.31 ± 0.04	125.14 ± 0.21	3.41 ± 0.03	125.65 ± 0.19	3.48 ± 0.10	126.18 ± 0.14	3.53 ± 0.12
0.5000	125.01 ± 0.09	4.16 ± 0.03	125.52 ± 0.08	4.22 ± 0.12	126.00 ± 0.12	4.27 ± 0.06	126.52 ± 0.22	4.35 ± 0.13	127.08 ± 0.25	4.43 ± 0.01

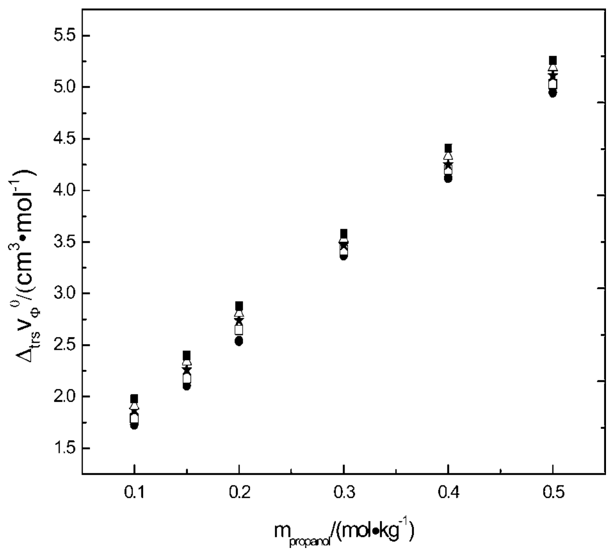

Figure 1. Variation of limiting partial molar volume of transfer of hexane-1,2,3,4,5,6-hexol, $\Delta_{trs}V^0_\Phi$, versus the molality of 1-propanol in aqueous solution at ●, 293.15 K; □, 298.15 K; ★, 303.15 K; △, 308.15 K; and ■, 313.15 K (since the tendency of $\Delta_{trs}V^0_\Phi$ versus the molality of 2-propanol is very close to 1-propanol, $\Delta_{trs}V^0_\Phi$ against molality of 2-propanol can be omitted).

peded; in other words, the hydroxyl group of 2-propanol cannot play its role thoroughly. Therefore, the values of $\Delta_{trs}V^0_\Phi$ for the hexane-1,2,3,4,5,6-hexol are smaller in the process of the polyol molecules transferring from water to water−2-propanol solvent mixtures.

Temperature Effect. Earlier reports clarified that group contributions of −OH in volume increase with the ascent of temperature.[29] On the other hand, an increase in temperature weakens the electrostriction. Both factors make the V^0_Φ increase with the increase in temperature. The data in Table 2 also indicate that V^0_Φ of hexane-1,2,3,4,5,6-hexol increases with the ascent of temperature, however, anomalies from $\Delta_{trs}V^0_\Phi$ only slightly increase with increase of temperature. The reason is maybe that V_Φ of hexane-1,2,3,4,5,6-hexol is increasing in both the water and the aqueous solutions of propanol with the increasing temperature, but the hydrophobic hydration gives some negative volume contribution to the whole system in the aqueous solutions of propanol, so it decreases the difference of V_Φ and V^0_Φ between hexane-1,2,3,4,5,6-hexol and water. At last, it makes the temperature effect on $\Delta_{trs}V^0_\Phi$ very weak.

Refractive Index and Molar Refractive Index. The refractive index (n_D) was directly related to the interactions in the solution. The data of n_D were used to calculate molar refractivity, R_D, with the Lorentz−Lorenz equation.[30]

$$R_D = [(n_D^{\ 2} - 1)/(n_D^{\ 2} + 2)]\left(\sum_{i=1}^{3} x_i M_i/\rho\right) \qquad (5)$$

where x_i and M_i are the mole fraction and molecular mass of the i-th component of the mixture. Equation 5 can be changed into eq 6 for data processing in this work:

$$R_D = M_1/\rho[(n_D^{\ 2} - 1)/(n_D^{\ 2} + 2)](1 + m_2M_2 + m_3M_3)/(1 + m_2M_1 + m_3M_1) \qquad (6)$$

where M_1, M_2, and M_3 respectively represent the molar mass of water, propanol, and hexane-1,2,3,4,5,6-hexol; m_2 and m_3 are the corresponding molarities of propanol and hexane-1,2,3,4,5,6-hexol.

The calculated values of R_D (298.15 K) along with the directly measured data of n_D are listed in Table 1. The variation of R_D at T = 298.15 K, as a function of hexane-1,2,3,4,5,6-hexol concentra-

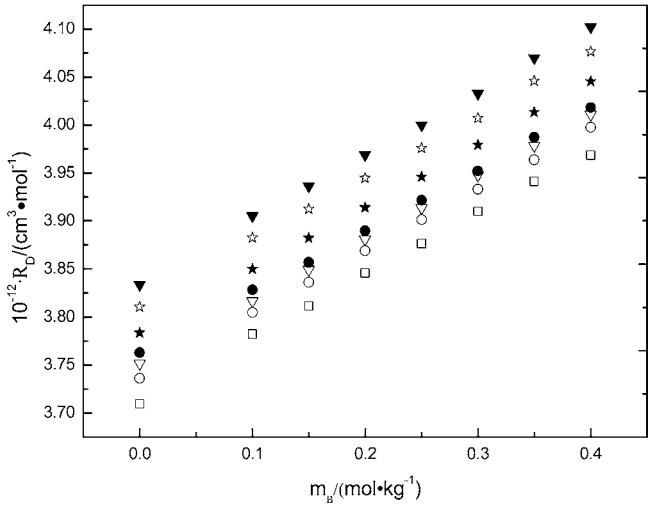

Figure 2. Variation of molar refractive index, R_D, versus the molality of hexane-1,2,3,4,5,6-hexol in an aqueous solution of 1-propanol at different concentrations at 298.15 K. □, pure water; ○, $m_{1\text{-propanol}} = 0.10$ mol·kg^{-1}; ▽, $m_{1\text{-propanol}} = 0.15$ mol·kg^{-1}; ●, $m_{1\text{-propanol}} = 0.20$ mol·kg^{-1}; ★, $m_{1\text{-propanol}} = 0.30$ mol·kg^{-1}; ☆, $m_{1\text{-propanol}} = 0.40$ mol·kg^{-1}; ▼, $m_{1\text{-propanol}} = 0.50$ mol·kg^{-1} (since the tendency of R_D versus molality of hexane-1,2,3,4,5,6-hexol in aqueous solution of 2-propanol is very close to 1-propanol, R_D against the molality of hexane-1,2,3,4,5,6-hexol in an aqueous solution of 2-propanol can be omitted).

tion, is depicted graphically in Figure 2. Single temperature plots have been given because there is not much variation in R_D within the experimental temperature range. The plots in Figure 2 are found to increase linearly with the increase in the relative amount of the solute. Since R_D is directly proportional to the molecular polarizability, the tendency in Figure 2 reveals that the overall polarizability of the ternary systems becomes stronger with the increase in the relative amount of hexane-1,2,3,4,5,6-hexol in the mixture. This may elucidate the structural cause of the change tendency of the density of the solution or the apparent molar volume of hexane-1,2,3,4,5,6-hexol (V_Φ) with the change in concentration of the polyol.

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