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ENTHALPIES OF MIXING AND APPARENT MOLAR VOLUMES OF ETHANOL SOLUTION OF CHIRAL DICARBOXYLIC ACIDS

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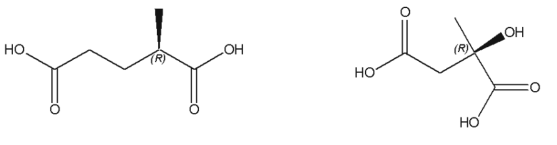
Enthalpies of mixing of *R*- and *S*-enantiomers of dicarboxylic acids such as 2-methylbutanedioic acid (MBA), 2-hydroxylbutanedioic acid (HBA), 2-methylpentanedioic acid (MPA) and 2-hydroxyl-2-methylbutanedioic acid (HMBA) in ethanol solution have been measured for a large range of mole fraction of heterochiral dicarboxylic acid at 298.15 K. Also densities of ethanol solution of the dicarboxylic acids were determined. Enthalpies of mixing were exothermic for all the concentrations. Enthalpic stabilization on mixing was increased with decreasing concentration of all dicarboxylic acids measured. Sequence of enthalpic stabilization on mixing was MBA<DHBA<MPA<HMBA<HBS at 0.5 mass%.

Keywords: *apparent molar volume, chiral compound, enthalpy of mixing, ethanol solution, 2-hydroxylbutanedioic acid, 2-hydroxyl-2-methylbutanedioic acid, 2-methylbutanedioic acid, 2-methylpentanedioic acid, R- and S-enantiomers*

Introduction

Enantiomers are unique molecules that have extensive effects throughout several aspects of organic chemistry, biology and pharmacology. The human body being amazingly chiral selective, will interact with each racemic drug differently and metabolize each enantiomers by a separate pathway to produce different pharmacological activity. Thus, one isomer may produce the desired therapeutic activities, while the other may be inactive or, in worst cases, produce unwanted effects. As a result chiral drugs have generated considerable interest in recent times. Hence physicochemical studies of model compounds in solutions are of fundamental importance in understanding the different aspects of chiral compounds. Takagi *et al.* [1] first measured the enthalpies of mixing of enantiomers of 2,3-dihydroxylbutanedioic acid (DHBA) followed by threonine and alanine. In recent years some investigators have studied the problem of chiral interaction [2–5]. Previous calorimetric work in our laboratory includes measurement of enthalpies of mixing for binary liquid chiral systems [6–11]. All observed systems showed a very small enthalpy change. Three systems were slightly exothermic showing slight enthalpic stabilization, whereas other eight systems were endothermic, showing a small enthalpic destabilization on mixing at 298.15 K. The intermolecular interactions between hetero chiral compounds were discussed. However there is very little literature on the mixing enthalpies in solution. Excess enthalpies of aqueous and ethanol solution of DHBA were observed for three different concentrations of aqueous and ethanol solutions of DHBA [10]. Enthalpies of mixing were exothermic for all the concentrations in both solvents. Enthalpic stabilization on mixing was increased with decreasing concentration of DHBA for both solvents. In order to understand enthalpic chiral discrimination of carboxylic acids in the solution, excess enthalpies of mixing of dicarboxylic acids of 2-methylbutanedioic acid (MBA), 2-hydroxylbutanedioic acid (HBA), 2-methylpentanedioic acid (MPA), 2-hydroxyl-2-methylbutanedioic acid (HMBA) shown in Fig. 1, have been measured in ethanol solution for a large range of mole fraction of heterochiral carboxylic acids at 298.15 K.

2-methylbutanedioic acid (MBA)
2-hydroxylbutanedioic acid (HBA)



2-methylpentanedioic acid (MPA)
2-hydroxyl-2-methylbutanedioic acid (HMBA)

Fig. 1 Structures of enantiomers(*R*-form)

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Experimental

R- and *S*-MBA, HBA, MPA, HMBA which supplied by Tokyo Chemical Industry or ALDRICH Chemical were used. Purity analysis by DSC showed 99.9 mole% or more. Ethanol (Kishida Kagaku, Special grade) was distilled and dried by storage over molecular sieves 4A freshly activated. Their chemical purities obtained from gas chromatography by using each 2 m column of 10% SE-30 on chromosorb and 20% PEG-1000 on celite 545 with FID on Yanagimoto G180FP are more than 99.99%. Water contents obtained by a coulometric Karl-Fischer's method on a Moisturemeter (Mitsubishi Chemical Ind., CA-02) was less than 0.001 mole%.

The excess enthalpies of mixing and dilution were measured by a microcalorimeter (Thermometric AB, Järfälla, Sweden) with a 0.8 mL mixing vessel at 298.15 K [12, 13]. Solutions of one enantiomer were placed in the stainless steel mixing vessel. The calorimeter syringe was filled with ca.500 μL solution of other enantiomers and placed in a pump. A cannula from the syringe was carefully inserted into the sample stage. Samples (20 to 100 μL) were injected into the vessel by use of gas-tight syringes (Hamilton 1710 or 1725N) fitted with stainless steel cannula (i.d. 0.2 mm, o.d. 0.45, length 1 m). Once assembled, the sample was left for about 2 h to equilibrate thermally. When it reached equilibrium temperature, the injection experiments were initiated. Details of the calorimetric procedure have been described previously [12, 13]. The enthalpies of solution of propane-1-ol in water was used as a test reaction [14] for the calorimetric measurements. Also other reliability test of the microcalorimeter system and the procedures used had been performed using a binary mixture of (1–*x*)1,4-dimethylbenzene+*x*1,3-dimethylbenzene and (1–*x*)1,4-dimethylbenzene and *x*1,2-dimethylbenzene as reported previously [14] for exothermic and endothermic system. Densities of the samples have been measured by a vibrating-tube densimeter (Anton Paar DMA60) at (298.15±0.001) K. The details of densitometric procedures were the same as those described previously [15].

Results and discussion

Experimental results of densities and molar volumes were shown in Table 1 and Fig. 2. Molar volumes of solutions of *R*- and *S*-dicarboxylic acids measured were determined with the smoothing Eq. (1):

$$V/\mathrm{cm}^3\mathrm{mol}^{-1}=a+bx \tag{1}$$

Table 1 Densities and molar volumes of ethanol solution of dicarboxylic acids at 298.15 K

R-dicarboxylic acid				*S*-dicarboxylic acid			
m/mol kg^{-1}	$10^3\ xR$	ρ/g cm^{-3}	V/cm^{-3}mol^{-1}	m/mol kg^{-1}	10^3xS	ρ/g cm^{-3}	V/cm^{-3}mol^{-1}
2-hydroxylbutanedioic acid							
0.037938	1.7609	0.78740	59.248	0.038334	1.7793	0.78747	59.245
0.075703	3.5077	0.78948	59.286	0.076178	3.5296	0.78956	59.282
0.15297	7.0626	0.79382	59.354	0.15348	7.0858	0.79388	59.352
0.22850	10.513	0.79804	59.419	0.23058	10.608	0.79812	59.423
2-methylbutanedioic acid							
0.036759	1.7063	0.78672	59.289	0.037344	1.7334	0.78677	59.288
0.077371	3.5847	0.78821	59.361	0.076366	3.5378	0.78836	59.364
0.15408	7.1133	0.79158	59.510	0.15574	7.1895	0.79175	59.505
0.23684	10.892	0.79551	59.660	0.23706	10.902	0.79527	59.662
2-methylpentanedioic acid							
0.036120	1.6767	0.78680	59.310	0.036413	1.6903	0.78668	59.311
0.068764	3.1872	0.78824	59.392	0.069265	3.2103	0.78838	59.385
0.14013	6.4734	0.79217	59.571	0.14057	6.4935	0.79127	59.581
0.21287	9.8011	0.79424	59.773	0.21297	9.8056	0.79432	59.768
2-hydroxyl-2-methylbutanedioic acid							
0.033506	1.5556	0.78714	59.273	0.033305	1.5462	0.78714	59.271
0.068424	3.1715	0.78902	59.339	0.068385	3.1697	0.78902	59.339
0.13866	6.4059	0.79600	59.448	0.13874	6.4098	0.79633	59.448
0.19968	9.1992	0.79666	59.589	0.20229	9.3186	0.79689	59.579

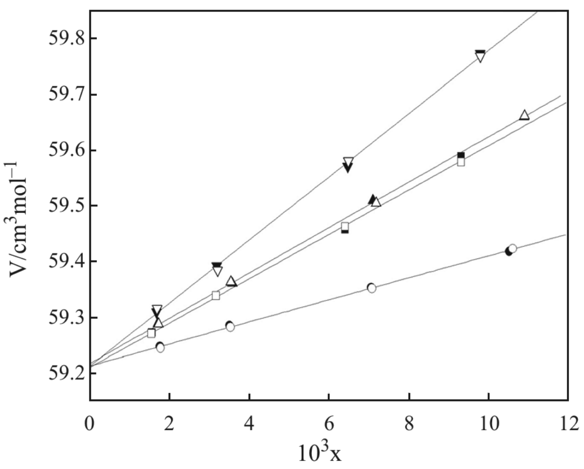

Fig. 2 Molar volumes of ethanol solutions of chiral dicarboxylic acids at 298.15 K: ● – *R*-HBA; ○ – *S*-HBA; ▲ – *R*-MBA; △ – *S*-MBA; ▼ – *R*-MPA; ▽ – *S*-MPA; ■ – *R*-HMBA; □ – *S*-HMBA

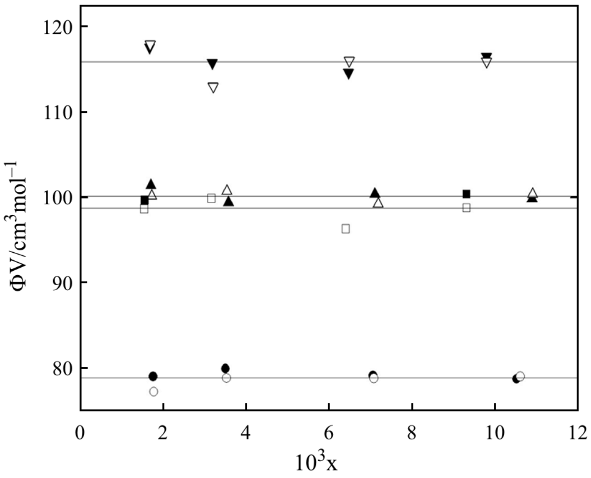

Fig. 3 Apparent molar volumes of ethanol solutions of chiral dicarboxylic acids at 298.15 K: ● – R-HBA; ○ – S-HBA; ▲ – *R*-MBA; △ – S-MBA; ▼ – *R*-MPA; ▽ – *S*-MPA; ■ – *R*-HMBA; □ – *S*-HMBA

where x is the mole fraction of dicarboxylic acids. Molar volumes of ethanol solution of *R*-dicarboxylic acid and *S*-dicarboxylic acid increased linearly with increasing concentration of dicarboxylic acids as shown in the Fig. 2. Those correlation coefficients were more than 0.999. When molar volumes of solution are extrapolated to x=1 by Eq. (1) with coefficients in Table 2, the values might be shown partial molar volumes of dicarboxylic acids in liquid state when excess volumes of mixing were zero. Apparent molar volumes φV of dicarboxylic acids were also calculated by Eq. (2) and are shown in Fig. 3.

$$\varphi V/\mathrm{cm}^3\ \mathrm{mol}^{-1}=(V–V_1^{*}n_1)/n_2 \qquad (2)$$

where V, V_1^*, n_1 and n_2 are molar volume of solution, volume of pure solvent, mole of ethanol and dicarboxylic acids, respectively. Apparent molar volumes of dicarboxylic acids were almost constant in ethanol as shown in Fig. 3. And the partial molar volumes of dicarboxylic acids of liquid state and apparent molar volumes were almost same value for each solution. That might indicate that excess volumes of mixtures of ethanol + hypothetical liquid of dicarboxylic acids at 298.15 K were shown negligible small and/or in error of this precision of the densitometry within the concentration range studied.

Enthalpies of mixing of ethanol solution of chiral dicarboxylic acids have been measured for wide range of molar ratio of heterochiral dicarboxylic acids at 298.15 K. Experimental results for enthalpies of mixing of ethanol solution of chiral dicarboxylic acids from 0.5 to 3 mass% were shown in Table 3 and in Figs 4 to 7. All enthalpies of mixing were exothermic for wide range of molar ratio of heterochiral dicarboxylic acids.

The mixing process of the ethanol solution of *R*- and *S*-dicarboxylic acids showed a stabilization of heterochiral contacts compared to each homochiral one over the whole range of composition at 298.15 K. Excess enthalpies on mixing are less exothermic than those in higher concentration of dicarboxylic acids in solutions as shown in Figs 4 to 7. In the ethanol solution of dicarboxylic acids, three states might be changed on mixing. One is the ionization of dicarboxylic acid, the second is solvation of dicarboxylic acid and the third is formation of heterochiral contacts. Enthalpy of ionization and enthalpy of solvation were endothermic reaction and exothermic reaction, respectively. The ionization of dicarboxylic acids in

Table 2 Parameters of Eq. (1) and apparent molar volumes of ethanol solution of dicarboxylic acids at 298.15 K

dicarboxylic acids	a	b	$10^3\ s_f$	a+b	ϕV/cm^3 mol^{-1}	s_f(ϕV)/cm^3 mol^{-1}
HBS	59.213	19.75	2.2	78.96	78.9	0.8
MBA	59.217	40.71	2.8	99.93	100.2	0.7
MPA	59.212	56.67	1.6	115.88	115.9	1.6
HMBA	59.210	39.83	4.8	99.04	98.7	1.6

V /cm^3 mol^{-1}= a+ bx (1), ϕV, apparent molar volume at infinite dilution; s_f(ϕV), standard deviation of the fits ; HBA, 2-hydroxylbutanedioic acid; MBA, 2-methylbutanedioic acid; MPA, 2-methylpentanedioic acid; HMBA, 2-hydroxyl-2-methylbutanedioic acid

Table 3 Excess enthalpies of mixing of (1- *f*)*S*-enantiomer and (*f*)*R*-enantiomers ethanol solution at 298.15 K

f	H^E/J mol^{-1}	f	H^E/J mol^{-1}	f	H^E/J mol^{-1}	f	H^E/J mol^{-1}
0.5114% ethanol solution of 2-hydroxylbutanedioic acid							
0.1602	–118.2	0.4327	–312.2	0.5597	–307.6	0.8356	–124.1
0.2761	–199.0	0.4881	–346.4	0.6289	–268.8		
0.3639	–257.2	0.5042	–345.4	0.7177	–214.6		
1.011% ethanol solution of 2-hydroxylbutanedioic acid							
0.1608	–50.79	0.4340	–133.3	0.5639	–139.1	0.8380	–54.74
0.2771	–87.06	0.4894	–150.6	0.6329	–118.2		
0.3651	–113.4	0.5085	–153.9	0.7212	–92.25		
1.921% ethanol solution of 2-hydroxylbutanedioic acid							
0.1630	–23.72	0.4380	–56.22	0.5643	–57.47	0.8382	–23.11
0.2804	–41.07	0.4934	–63.87	0.6333	–50.07		
0.3688	–48.73	0.5089	–63.82	0.7215	–38.13		
2.999 % ethanol solution of 2-hydroxylbutanedioic acid							
0.1611	–17.06	0.4345	–42.41	0.5661	–40.67	0.8392	–15.42
0.2775	–29.16	0.4899	–46.77	0.6350	–34.48		
0.3656	–36.52	0.5107	–44.96	0.7230	–27.14		
0.4910 % ethanol solution of 2-methylbutanedioic acid							
0.1597	–72.64	0.4320	–176.5	0.5569	–169.2	0.8341	–69.95
0.2755	–118.4	0.4873	–196.0	0.6262	–144.8		
0.3632	–150.7	0.5013	–191.1	0.7154	–114.3		
0.9987% ethanol solution of 2-methylbutanedioic acid							
0.1612	–39.29	0.4346	–104.2	0.5670	–103.4	0.8397	–38.43
0.2776	–66.82	0.4900	–115.9	0.6358	–88.45		
0.3657	–89.04	0.5116	–117.7	0.7236	–65.93		
2.016% ethanol solution of 2-methylbutanedioic acid							
0.1608	–20.44	0.4338	–54.46	0.5613	–53.70	0.8365	–21.58
0.2770	–36.07	0.4892	–60.57	0.6304	–45.82		
0.3650	–46.29	0.5058	–60.01	0.7190	–35.67		
3.037% ethanol solution of 2-methylbutanedioic acid							
0.1660	–8.010	0.4432	–20.38	0.5625	–20.16	0.8372	–7.640
0.2847	–13.49	0.4988	–22.79	0.6315	–17.02		
0.3738	–17.26	0.5070	–22.47	0.7200	–12.76		
0.5293% ethanol solution of 2-methylpentanedioic acid							
0.1627	–93.83	0.4373	–246.5	0.5612	–247.4	0.8365	–96.70
0.2798	–158.2	0.4927	–276.4	0.6304	–210.5		
0.3682	–208.9	0.5057	–276.6	0.7190	–162.7		
1.002% ethanol solution of 2-methylpentanedioic acid							
0.1622	–49.72	0.4364	–132.3	0.5600	–134.5	0.8358	–50.63
0.2791	–85.88	0.4919	–150.0	0.6292	–113.4		
0.3674	–113.2	0.5045	–150.9	0.7179	–86.56		
2.013% ethanol solution of 2-methylpentanedioic acid							
0.1652	–26.54	0.4418	–63.89	0.5612	–62.35	0.8365	–26.32
0.2835	–42.66	0.4973	–69.97	0.6303	–54.67		
0.3724	–54.29	0.5057	–68.95	0.7189	–43.27		

Table 3 continued

f	H^E/J mol^{-1}	f	H^E/J mol^{-1}	f	H^E/J mol^{-1}	f	H^E/J mol^{-1}
3.020% ethanol solution of 2-methylpentanedioic acid							
0.1631	–16.50	0.4380	–43.05	0.5608	–42.83	0.8362	–16.18
0.2804	–28.20	0.4934	–48.40	0.6299	–36.22		
0.3689	–36.65	0.5053	–47.86	0.7186	–27.67		
0.5023% ethanol solution of 2-hydroxyl-2-methylbutanedioic acid							
0.1639	–121.1	0.4395	–286.1	0.5608	–286.3	0.8363	–121.5
0.2816	–203.5	0.4950	–307.5	0.6299	–251.4		
0.3703	–251.3	0.5053	–307.4	0.7186	–204.3		
1.003% ethanol solution of 2-hydroxyl-2-methylbutanedioic acid							
0.1635	–57.08	0.4387	–132.7	0.5622	–131.4	0.8370	–56.12
0.2810	–92.57	0.4942	–142.3	0.6313	–116.3		
0.3696	–117.7	0.5067	–140.8	0.7197	–91.53		
2.013% ethanol solution of 2-hydroxyl-2-methylbutanedioic acid							
0.1649	–26.89	0.4412	–64.05	0.5592	–63.22	0.8354	–26.91
0.2831	–45.28	0.4968	–69.32	0.6285	–56.11		
0.3720	–56.08	0.5037	–68.45	0.7173	–45.26		
2.993% ethanol solution of 2-hydroxyl-2-methylbutanedioic acid							
0.1649	–19.03	0.4414	–43.65	0.5588	–43.65	0.8352	–18.54
0.2832	–30.39	0.4969	–47.71	0.6281	–38.23		
0.3721	–38.22	0.5033	–47.81	0.7170	–30.41		

n_R : Mole of *R*-enantiomer, n_S : Mole of *S*-enantiomer, $f = n_R / (n_R + n_S)$, $H^E = Q_{total} / (n_R + n_S)$

ethanol solution might be very small. Then the effect of the enthalpy of ionization of dicarboxylic acids on enthalpy of mixing might be negligible. Accessible surface areas and volumes of dicarboxylic acids calculated by HyperChem [16] were shown in Table 5. Here van der Waals volume of ethanol molecule was calculated 0.05263 nm^3. From this radius of ethanol was 232.5 pm as a sphere shape molecule. Geometry optimization of molecular shapes of dicarboxylic acids were carried out by calculations using the AM1 method [17, 18] and shown in Table 4. Surface fractions *s*=ASA (dicarboxylic acid)/{ASA(dicarboxylic acid)+ASA(ethanol)} of solutions observed were less than 0.02. Surface fractions are corresponding to site fractions. So molecules of dicarboxylic acids in ethanol solution may not contact directly, because dicarboxylic acids may strongly solvate with ethanol. The solutions measured might have enough amounts of ethanol to make the first solvated shell in this work.

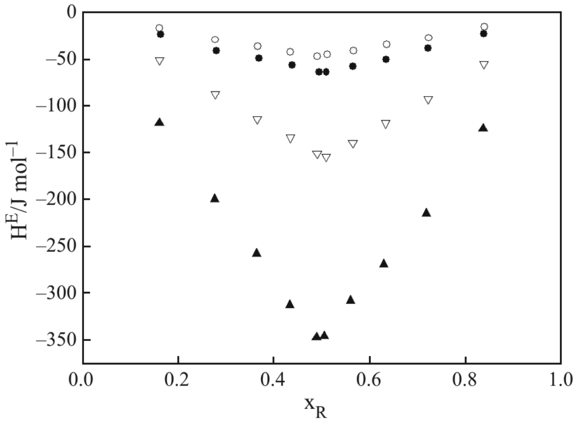

Fig. 4 Excess enthalpies of ethanol solution of *R*- and S-HBA at 298.15 K: ▲ – 0.5 mass% ethanol solution; ▽ – 1 mass% ethanol solution; ● – 2 mass% ethanol solution; ○ – 3 mass% ethanol solution

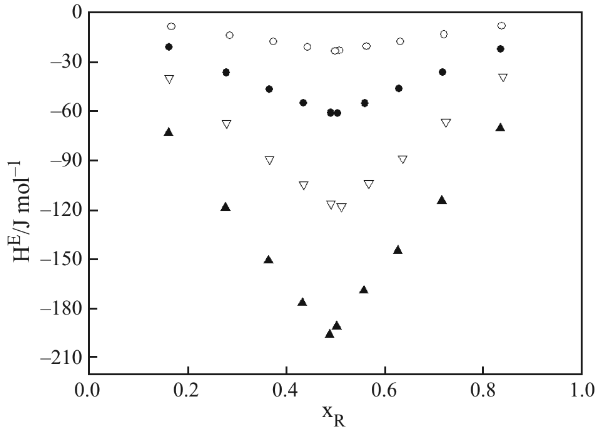

Fig. 5 Excess enthalpies of ethanol solution of *R*- and *S*-MSA at 298.15 K: ▲ – 0.5 mass% ethanol solution; ▽ – 1 mass% ethanol solution; ● – 2 mass% ethanol solution; ○ – 3 mass% ethanol solution

Table 4 van der Waals volumes, accessible volumes and accessible surface areas of dicarboxylic acids and ethanol

	VDW/nm^3	AV/nm^3	ASA/nm^2	AV_{DA}/AV_{EtOH}	ASA_{DA}/ASA_{EtOH}
EtOH	0.05263	0.4702	3.299		
DHBA	0.1083	0.7387	3.315	1.571	1.005
HBS	0.1014	0.7095	3.583	1.509	1.086
MBA	0.1120	0.7525	4.119	1.600	1.249
MPA	0.1288	0.8424	4.500	1.792	1.364
HMBA	0.1182	0.7723	3.817	1.643	1.157

VDW: van der Waals volume; AV and ASA: accessible volume and accessible surface area which estimated by probe of 232.5 pm. Subscript DA means dicarboxylic acid HBA, 2-hydroxylbutanedioic acid; MBA, 2-methylbutanedioic acid; MPA, 2-methylpentanedioic acid; HMBA, 2-hydroxyl-2-methylbutanedioic acid; DHBA, 2,3-dihydroxylbutanedioic acid

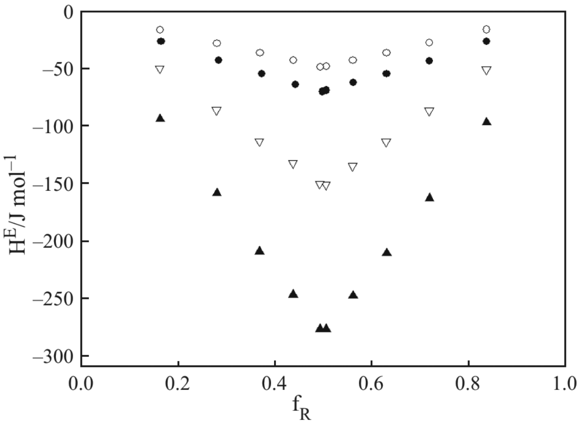

Fig. 6 Excess enthalpies of ethanol solution of *R*- and *S*-MPA at 298.15 K: ▲ – 0.5 mass% ethanol solution; ▽ – 1 mass% ethanol solution; ● – 2 mass% ethanol solution; ○ – 3 mass% ethanol solution

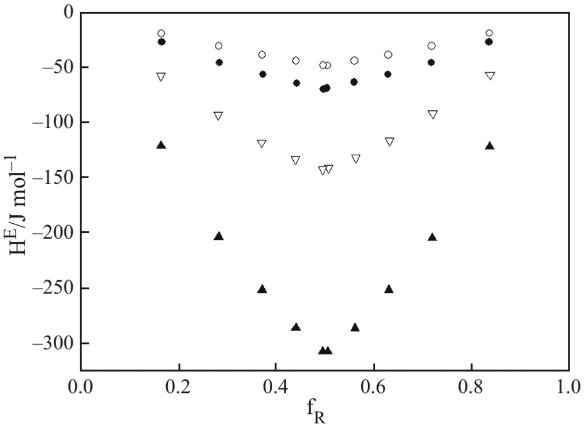

Fig. 7 Excess enthalpies of ethanol solution of *R*- and S-HMBA at 298.15 K: ▲ – 0.5 mass% ethanol solution; ▽ – 1 mass% ethanol solution; ● – 2 mass% ethanol solution; ○ – 3 mass% ethanol solution

The solvated ethanol in the first solvation shell of *R*- and *S*-dicarboxylic acids solution might be strongly oriented to each enantiomers. In the case of dilute solution, there was also a possibility of relatively strong solvation to first solvation shell. But for the higher concentrations, the possibility might be decreased with increasing concentration of dicarboxylic acids. The one of the major reason is that the amounts of solvent around the first shell are not in sufficient quantity. That might be the reason for less stability of mixing for higher concentration. As results, exothermic enthalpy changes were decreased with increasing concentration of dicarboxylic acids. According to the results of X-ray analysis of the solution [18] and molecular dynamic simulation [19], there are many solvent between dicarboxylic acids in solution. The solvents in the first solvated shell may strongly orient around dicarboxylic acids. When solutions of each enantiomers were mixed, the configuration of solvents in the second shell around the dicarboxylic acids might change largely. Because the orientation of solvents might be not as strong as the solvent in the first shell.

Table 5 Excess enthalpies on mixing at $x=0.5$ for different concentrations, mass/mass% solutions

Dicarboxylic acids	H^E /J mol^{-1}			
sol./%	0.5	1	2	3
HBA	–348.6	–154.1	–64.39	–46.84
MBA	–196.6	–118.3	–61.05	–22.95
MPA	–278.6	–151.8	–70.58	–48.78
HMBA	–310.2	–143.4	–69.82	–48.19

HBA, 2-hydroxylbutanedioic acid; MBA, 2-methylbutanedioic acid; MPA, 2-methylpentanedioic acid; HMBA, 2-hydroxyl-2-methylbutanedioic acid

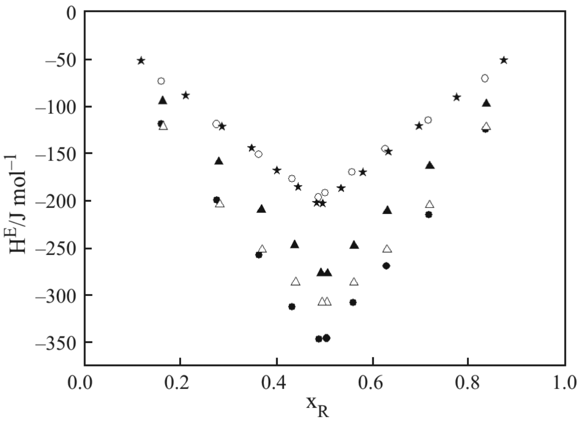

Fig. 8 Comparison of the enthalpies of mixing of enantiomers for dicarboxylic acids at 0.5% ethanol solutions : ● – HBS; ○ – MBA; ▲ – MPA; △ – HMBA; ★ – DHBA [10]

To compare interaction of the dicarboxylic acids in ethanol, excess enthalpies at 0.5 mass% ethanol solutions of MBA, HBA, MPA, HMBA and DHBA were shown in Fig. 8. Sequence of stabilization on mixing at equimolar mixtures of heterochiral dicarboxylic acids were following:

MBA<DHBA<MPA<HMBA<HBA

As shown in Table 5 and Fig. 8, enthalpies of mixing of MPA enantiomer were more stable compared to that of MBA. Similar comparison between HBA and that of HMBA showed HBA enantiomer's large stability compared to HMBA's enantiomer. The differences between these carboxylic acids are the substituent group at 2-carbon atom. Two acids have methyl group at 2-carbon atom and other two acids have hydroxyl group at the same position. Castronuovo *et al.* [21] were discussed about different capability of functional group for promoting hydrophobic interactions. The position of the functional groups also had meaningful significance. Upon the interaction between two hydrated molecules, the two carboxyl groups, placed at the opposite ends of the molecules, determine an attenuation of hydrophobic interactions probably caused by the steric hindrance of the carboxyl groups, an effect which decreases when the alkyl chain become longer [22]. On the other hand with respect to interaction between hydroxyl-hydroxyl and carboxyl-carboxyl, the hydroxyl-carboxyl interaction might be responsible for more effectively to the overlapping of hydrophobic hydration co-spheres. This could be due to the relative compatibility of the geometries of the hydrated carboxyl and hydroxyl groups leading to the enhanced cooperatively of hydrophobic interactions sustained by hydroxyl-carboxyl hydrophilic interactions [20]. In the present study among the two hydroxyl acids, HMBA is less stable. This may be due to steric hindrance caused by the presence of methyl group in the same carbon atom with hydroxyl group. In our previous paper [10], we have reported the results for similar experiments with DHBA. Comparing the result of DHBA with the dicarboxylic acids studied in this work, Fig. 8 showed that mixing of DHBA enantiomers were thermodynamically less stable compared to other hydroxyl acids studied. In DHBA two carboxyl and two hydroxyl groups are very close to each other. That might decrease the effective overlap of hydrophobic domain of DHBA making the mixing process less stable.

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