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By

Chandrakant S. Aher

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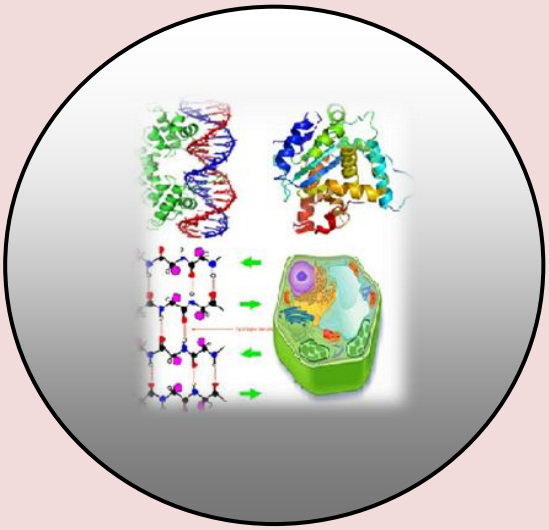

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Dr. C. S. Aher
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Solubility, Density and Thermodynamic Functions of Catechol in Pure Water, 1-Propanol and Their Binary Solvent Mixtures at 293.15 to 313.15 K Temperatures

Chandrakant S. Aher
Department of Chemistry, M.S.G. College Malegaon Camp, Pin 423105. India

ABSTRACT

Solubility of catechol in water, 1-propanol and in water+1-propanol binary mixtures have been experimentally measured using a gravimetric method at temperatures (293.15, 295.15, 298.15, 300.15, 303.15, 305.15, 308.15, 310.15 & 313.15) K. Catechol solubility values are correlated with temperature by using the Apelblat equation. The combined nearly ideal binary solvent (NIBS)-Redlich-Kister equation is used to fit experimental solubility data in mixed solvents at constant temperature. The modified van't Hoff equation is used to obtained thermodynamic functions including ΔH^0_{soln}, ΔG^0_{soln}, and ΔS^0_{soln} of catechol in different solvents.

Keyword: Solubility, Catechol, NIBS, Density, van't Hoff equation and Apelblat equation.

INTRODUCTION

Fruits and vegetables are natural source of catechol in small amount; it is one of the main natural phenols in argan oil (Zheng et al, 2008). Solubility data is required for selection of proper solvent and design an optimized crystallization process, solubility of catechol in pure solvents for some temperatures are available (Stephan H. and Stephen T., 1963). But there are no data available on solubility of catechol in water+1-propanol for the complete binary composition range. In this paper the systematic study of solubility and density of catechol in water + 1-propanol binary solvents over the entire composition range from 0 to 1 mole fraction, at temperatures (293.15 to 313.15) K is reported. The thermodynamic functions for saturated catechol solution are calculated using modified van't Hoff equation.

MATERIALS AND METHOD

Material

Triple distilled water was used in all experiments. Other chemicals was supplied by

Chemical Name	Supplier Name	Percentage purity	Standard
Catechol	Sigma-Aldrich co.	≥99%	Reagent Grade
1-Propanol	Spectrochem Pvt. Ltd, Mumbai, India.	≥99.8%	HPLC

Apparatus and Procedure

The solubility of catechol is measured using an apparatus similar to that described in the literature (Pawar et al 2012, Pawar et al 2009, Pawar et al 2010). In this work, an excess amount of catechol was added to the binary solvents mixtures prepared by weight (Shimadzu, Auxzzo) with an uncertainty of ± 0.1 mg, in a specially designed 100 ml double jacketed flask. Water was circulated at constant temperature in jacket between the outer and inner walls of the flask. Densities were determined using a 15 cm^3 bicapillary pycnometer, these data are used to explained excess functions as described earlier. (Kadam et al, 2006, Hasan et al, 2006, Marsh K. N. 1987, Pawar R.R. and Aher C. S. 2017, Pawar R.R. and Aher C. S. 2017, Pawar R.R. and Aher C. S. 2017, Pawar R.R. and Aher C. S. 2018).

RESULTS AND DISCUSSION

Solubility: Table 1 show the experimental and calculated (using Apelblat equation) values of solubility (x_B) of catechol at 293.15 to 313.15 K in water, 1-propanol and water + 1- propanol respectively. The density of saturated solution is also reported. Variation of solubility with x_C^0 is visually shown in Fig. 1.

Table 1-Experimental $x_{B(exp.)}$ and Calculated $x_{B(cal.)}$ Values of Mole Fraction Solubility and Density (ρ) of Catechol for Various Initial Mole Fractions, (x_C^0), of 1-Propanol at Temperatures (293.15 to 313.15) K and Pressure 101.32 kPa^a.

T/(K)	x_C^0	$x_{B(exp.)}$	$x_{B(cal.)}$	RD	$\rho\ 10^{-3}/kg\ m^{-3}$
293.15	0.0000	0.0752	0.0749	0.0048	1.0732
	0.1000	0.1897	0.1887	0.0052	1.0942
	0.2001	0.2418	0.2412	0.0023	1.0826
	0.2999	0.2774	0.2765	0.0032	1.0698
	0.4001	0.2999	0.3006	0.0021	1.0562
	0.5000	0.3201	0.3182	0.0058	1.0445
	0.6000	0.3169	0.3187	0.0058	1.0326
	0.6998	0.3422	0.3417	0.0014	1.0209
	0.8002	0.3480	0.3492	0.0036	1.0101
	0.8999	0.3498	0.3515	0.0049	0.9999
	1.0000	0.3355	0.3407	0.0157	1.0224
295.65	0.0000	0.0888	0.0895	0.0078	1.0828
	0.1000	0.1996	0.2008	0.0057	1.0970
	0.2001	0.2498	0.2510	0.0045	1.0845
	0.2999	0.2845	0.2868	0.0080	1.0712
	0.4001	0.3102	0.3095	0.0023	1.0580
	0.5000	0.3268	0.3259	0.0027	1.0454
	0.6000	0.3297	0.3286	0.0032	1.0342
	0.6998	0.3488	0.3492	0.0012	1.0227
	0.8002	0.3578	0.3566	0.0034	1.0116
	0.8999	0.3623	0.3608	0.0042	1.0015
	1.0000	0.3566	0.3518	0.0137	1.0236
298.15	0.0000	0.1036	0.1057	0.0201	1.0911
	0.1000	0.2125	0.2132	0.0033	1.0999
	0.2001	0.2609	0.2614	0.0020	1.0870
	0.2999	0.2985	0.2972	0.0044	1.0734
	0.4001	0.3181	0.3188	0.0023	1.0600
	0.5000	0.3294	0.3340	0.0139	1.0478
	0.6000	0.3419	0.3386	0.0097	1.0359
	0.6998	0.3562	0.3573	0.0031	1.0239
	0.8002	0.3659	0.3646	0.0035	1.0130
	0.8999	0.3714	0.3700	0.0038	1.0027
	1.0000	0.3666	0.3625	0.0109	1.0256

300.65	0.0000	0.1263	0.1232	0.0242	1.0997
	0.1000	0.2265	0.2260	0.0022	1.1039
	0.2001	0.2734	0.2725	0.0033	1.0899
	0.2999	0.3074	0.3079	0.0015	1.0762
	0.4001	0.3301	0.3287	0.0041	1.0615
	0.5000	0.3379	0.3426	0.0137	1.0493
	0.6000	0.3479	0.3487	0.0024	1.0372
	0.6998	0.3665	0.3660	0.0011	1.0261
	0.8002	0.3722	0.3731	0.0024	1.0152
	0.8999	0.3803	0.3792	0.0029	1.0049
	1.0000	0.3746	0.3731	0.0041	1.0273
303.15	0.0000	0.1445	0.1420	0.0172	1.1089
	0.1000	0.2390	0.2392	0.0008	1.1068
	0.2001	0.2860	0.2844	0.0054	1.0923
	0.2999	0.3203	0.3187	0.0048	1.0789
	0.4001	0.3392	0.3390	0.0005	1.0642
	0.5000	0.3585	0.3516	0.0192	1.0512
	0.6000	0.3583	0.3589	0.0018	1.0389
	0.6998	0.3776	0.3754	0.0057	1.0289
	0.8002	0.3827	0.3822	0.0012	1.0174
	0.8999	0.3877	0.3884	0.0018	1.0071
	1.0000	0.3823	0.3833	0.0027	1.0291
305.65	0.0000	0.1621	0.1618	0.0018	1.1158
	0.1000	0.2533	0.2527	0.0022	1.1099
	0.2001	0.2973	0.2971	0.0008	1.0942
	0.2999	0.3301	0.3297	0.0012	1.0804
	0.4001	0.3513	0.3498	0.0042	1.0668
	0.5000	0.3621	0.3611	0.0027	1.0544
	0.6000	0.3680	0.3692	0.0032	1.0417
	0.6998	0.3839	0.3855	0.0040	1.0299
	0.8002	0.3914	0.3920	0.0015	1.0218
	0.8999	0.3949	0.3977	0.0070	1.0087
	1.0000	0.3899	0.3932	0.0085	1.0317
308.15	0.0000	0.1781	0.1823	0.0239	1.1224
	0.1000	0.2664	0.2666	0.0006	1.1126
	0.2001	0.3082	0.3106	0.0080	1.0969
	0.2999	0.3395	0.3410	0.0043	1.0826
	0.4001	0.3570	0.3612	0.0118	1.0681
	0.5000	0.3692	0.3711	0.0052	1.0560
	0.6000	0.3775	0.3796	0.0056	1.0419
	0.6998	0.3958	0.3963	0.0011	1.0320
	0.8002	0.4013	0.4024	0.0027	1.0227
	0.8999	0.4053	0.4069	0.0038	1.0111
	1.0000	0.3980	0.4028	0.0123	1.0340
310.65	0.0000	0.2003	0.2032	0.0144	1.1280
	0.1000	0.2823	0.2808	0.0055	1.1153
	0.2001	0.3252	0.3251	0.0001	1.1000
	0.2999	0.3514	0.3524	0.0027	1.0847
	0.4001	0.3740	0.3731	0.0024	1.0706

	0.5000	0.3854	0.3816	0.0099	1.0575
	0.6000	0.3921	0.3900	0.0052	1.0457
	0.6998	0.4084	0.4078	0.0016	1.0344
	0.8002	0.4136	0.4135	0.0004	1.0239
	0.8999	0.4196	0.4161	0.0085	1.0133
	1.0000	0.4131	0.4121	0.0024	1.0364
313.15	0.0000	0.2280	0.2241	0.0171	1.1328
	0.1000	0.2939	0.2953	0.0046	1.1184
	0.2001	0.3414	0.3405	0.0025	1.1024
	0.2999	0.3650	0.3640	0.0029	1.0873
	0.4001	0.3865	0.3856	0.0025	1.0728
	0.5000	0.3896	0.3927	0.0080	1.0603
	0.6000	0.4008	0.4006	0.0005	1.0480
	0.6998	0.4198	0.4200	0.0004	1.0365
	0.8002	0.4259	0.4252	0.0016	1.0264
	0.8999	0.4244	0.4252	0.0019	1.0157
	1.0000	0.4243	0.4210	0.0077	1.0396

[a]Standard uncertainties in u are u(T) = 0.1 K, u($x_C{}^0$) = 0.0002, u(x_B) = 0.003, and u(ρ) = 10 kg·m^{-3}. The relative uncertainty in pressure ur (p) = 0.05.

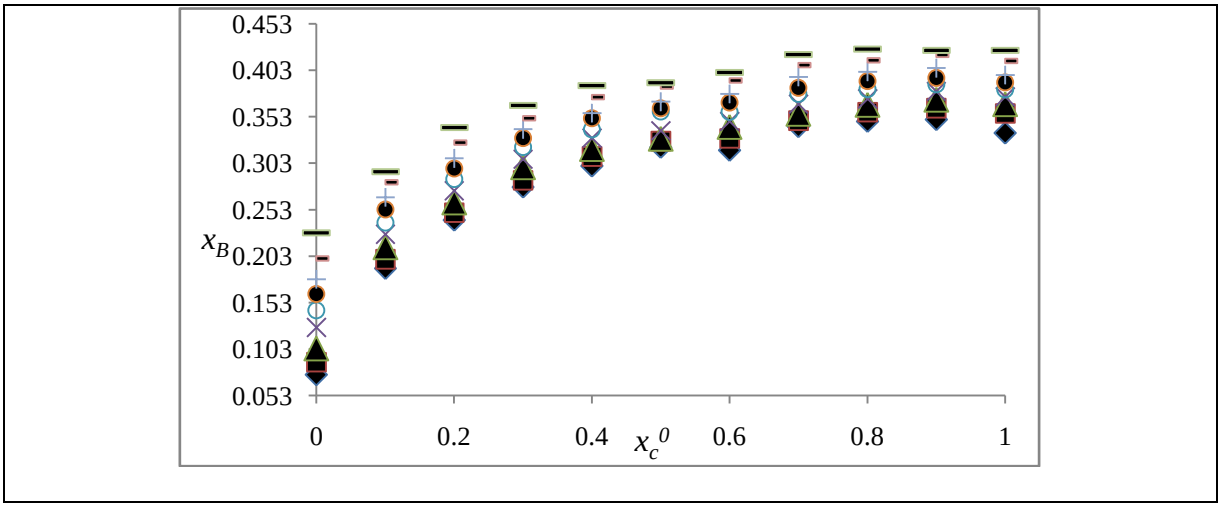

Figure 1. Mole Fraction Solubility (x_B) Variation with Initial Mole Fraction (x_C^0) of 1-Propanol at Various Temperatures (◆T=293.15 K, ■T=295.65 K; ▲T=298.15 K; ×T= 300.65 K; ○T=303.15K; ●T=305.65 K; +T=308.15 K; -T=310.65 K and —T=313.15 K).

The solubility of catechol in all solvents increases with temperature. At the same temperature, the solubility trend in solvent is 1-propanol > water + 1-propanol >water. This trend implies that solubility of catechol increases with increasing with mole fraction of 1-propanol, it is prefer to dissolve more in 1-propanol than water. The solubility of catechol in water+1-propanol mixture with x_C^0 increases with increases in x_B up x_C^0=1. This implies that there is strong dipole-dipole interaction between solute and solvent molecules.

Apelblat Model: The modified semi-empirical Apelblat model (eq 1) is a suitable method to correlate solubility data against temperature (Lourenço et al. 2012, Melo et al. 2013).

The equation is based on solid-liquid equilibrium theory provide excellent agreement between experimental and calculated values of solubility (Domańska U., Bogel-Łukasik R. 2005).

$$lnx_{B=} A + \frac{B}{T} + ClnT \qquad \ldots\ldots\ldots\ldots (1)$$

A, *B*, and *C* are the model parameters and T is temperature in Kelvin. *A* and *B* represent the non-idealities of the solutions in terms of the variation of activity coefficients, *C* reflects to the effect of temperature on the enthalpy of fusion (Apelblat A., Manzurola E. 1999). *A*, *B*, and *C* parameters are determined using non-linear least square fitting (Gans et al. 1996). Solubility values of catechol in water, methanol, and their mixtures are calculated by eq 1. Relative deviation (*RD)* (Guo et al. 2016) is calculated using eq 2.

$$RD = \frac{x_B^{exp.} - x_B^{cal.}}{x_B^{exp.}} \qquad \ldots\ldots\ldots\ldots\ldots (2)$$

The data of experimental mole fraction solubility, calculated solubility and *RD* in monosolvent (water, methanol) and water-methanol mixtures are listed in Table 1. The values of parameters *A*, *B*, *C* along with co-relation coefficient (R^2) are listed in Table 2.

Table 2. Model Parameters and Correlation Coefficient of the Apelblat Equation.

Solvents	**Mole fraction x_C^0**	**Parameters**			R^2
		A	*B*	*C*	
1-Propanol	0.0000	926.5154	-46178.9730	-135.8253	0.9971
	0.1000	78.1822	-5341.3275	-10.8489	0.9991
	0.2001	-161.7337	5893.9307	24.6812	0.9983
	0.2999	3.2809	-1273.3316	-0.0392	0.9971
	0.4001	-99.1287	3451.0944	15.1662	0.9955
	0.5000	-107.159	3966.755	16.28015	0.9767
	0.6000	11.8861	-1475.3680	-1.4077	0.9941
	0.6998	-152.1735	6016.6385	22.9859	0.9978
	0.8002	-137.8249	5406.7063	20.8301	0.9979
	0.8999	20.5386	-1712.8800	-2.7710	0.9919
	1.0000	107.5766	-5723.8774	-15.6896	0.9732

Table 3. NIBS-Redlich-Kister model parameters.

T/K	Range of x_C^0	M_0	M_1	M_2	M_3	R^2
Water + 1-Propanol + Catechol						
293.15	0.10-0.90	2.552	-1.679	4.141	-3.620	0.990
295.65	0.10-0.90	2.240	-1.538	3.439	-3.115	0.991
298.15	0.10-0.90	2.000	-1.417	3.035	-2.626	0.992
300.65	0.10-0.90	1.696	-1.235	2.405	-1.839	0.992
303.15	0.10-0.90	1.565	-1.083	1.932	-1.463	0.993
305.65	0.10-0.90	1.397	-0.960	1.708	-1.256	0.993
308.15	0.10-0.90	1.260	-0.798	1.606	-1.150	0.994
310.65	0.10-0.90	1.120	-0.742	1.299	-0.809	0.994
313.15	0.10-0.90	0.956	-0.660	0.758	-0.364	0.992

NIBS-Redlich-Kister Model

The solubility data at constant temperature is fitted into combined NIBS-Redlich-Kistermodel (Jouyban et al. 2002, Joyce et al. 1995, Acree W.E. and Zvaigzne A.I. 1991, Acree W. E. 1992).

$$lnx_B = x_C^0 lnx_1 + x_A^0 lnx_2 + x_C^0 x_A^0 \sum_{i=0}^{3} M_i \, (x_C^0 - x_A^0)^i \qquad \ldots\ldots\ldots (3)$$

Where x_A^0 is initial mole fraction of water and x_1, x_2 are solubilities of catechol in pure methanol and water, respectively. M_i is curve fit parameters (four parameter equation). All values of M_i along with R^2 value are listed in Table 3. The values of R^2 are close to unity shows that NIBS-Redlich-Kister model is very well applicable for this solubility data.

Table 5. Thermodynamic Functions Relative to Solution Process of Catechol at *Tmean* =302.928K

x_C^0	ΔH^0_{sol}/kJ K^{-1} mol^{-1}	ΔG^0_{soln}/kJ K^{-1} · mol^{-1}	ΔS^0_{soln}/KJ K^{-1} mol^{-1}	$T\Delta S^0_{soln}$/KJ K^{-1} mol^{-1}	%ζH	%ζTS
Water + 1-Propanol						
0.0000	41.8194	4.9954	121.4712	36.8240	53.18	46.82
0.1000	17.0437	3.6092	44.3164	13.4345	55.92	44.08
0.2001	13.1361	3.1530	32.9313	9.9831	56.82	43.18
0.2999	10.4756	2.8808	25.0531	7.5948	57.97	42.03
0.4001	9.4780	2.7170	22.3024	6.7610	58.37	41.63
0.5000	8.0238	2.6252	17.8084	5.3986	59.78	40.22
0.6000	8.6466	2.5809	20.0088	6.0657	58.77	41.23
0.6998	7.8152	2.4549	17.6820	5.3603	59.32	40.68
0.8002	7.4826	2.4120	16.7263	5.0706	59.61	40.39
0.8999	7.2332	2.3843	15.9950	4.8489	59.87	40.13
1.0000	8.0646	2.4246	18.6045	5.6400	58.85	41.15

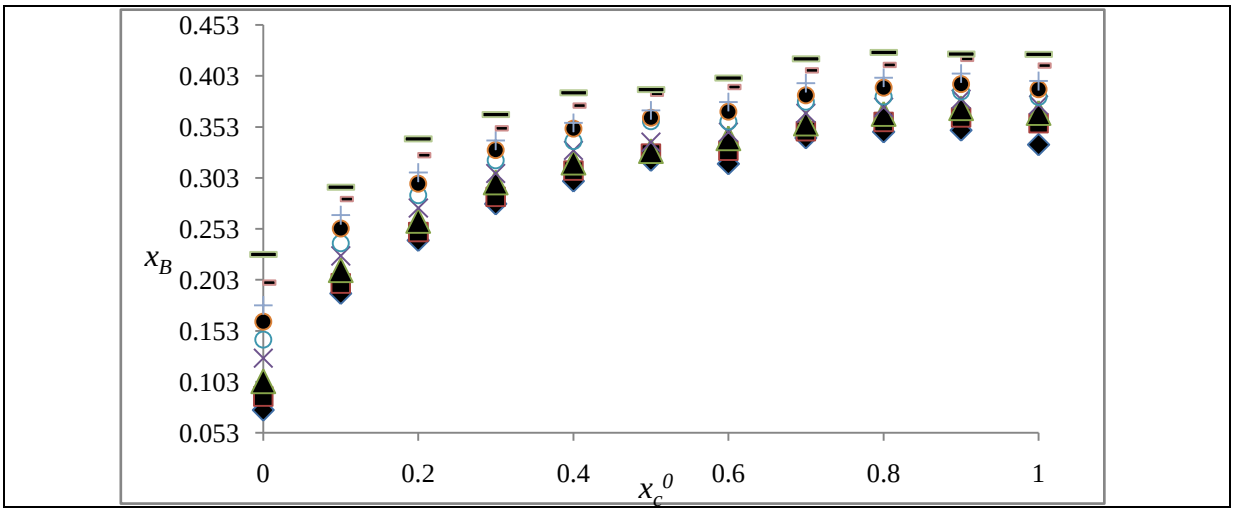

Figure 2. Mole Fraction Solubility (x_B) Variation with Initial Mole Fraction (x_C^0) of 1-Propanol at Various Temperatures (◆T=293.15 K, ■T=295.65 K; ▲T=298.15 K; ×T=300.65 K; ○T=303.15K; ●T=305.65 K; +T=308.15 K; -T=310.65 K and —T=313.15 K).

Thermodynamics Functions of Dissolution: According to the van't Hoff equation, the standard molar enthalpy change of solution ΔH^0_{soln} is generally obtained from the slope of the $ln\ x_B$ vs $1/T$ plot. Average temperature T_{mean} is introduced to obtain a single value of ΔG^0_{soln} and ΔS^0_{soln} in the temperature range studied.

$$T_{mean}\ \frac{n}{\sum_{i-1}^{n}\left(\frac{1}{T}\right)} \qquad \text{..... (4)}$$

Where n is the number of experimental points. In the present work, T_{mean} = 302.98 K and the temperature range is (293.15 to 313.15) K in both pure solvents and binary solvent mixtures. Heat capacity of the solution can be assumed as constant. Hence values of ΔH^0_{soln} are derived using eq 5.

$$\Delta H^0_{sol} = -R\left(\frac{\partial \ln x_B}{\partial\, 1/T}\right) - R\left[\frac{\partial \ln x_B}{\partial\left(\frac{1}{T}-\frac{1}{T_{mean}}\right)}\right] \qquad \text{……..(5)}$$

The lnx_B Vs 10000 $(1/T - 1/Tmean)$ plot of different solutions including pure solvents and binary solvent mixtures are displayed in Fig. 2. From these figures, it can be seen that a trend of increasing solubility with temperature is observed. The slope and the intercept for each solvent are listed in Table 4. Thus the modified van't Hoff equation can be thought to be fit to calculate the enthalpy change of solution. The standard molar Gibbs energy change for the solution process ΔG^0_{soln}, can be calculated in the way similar to Krug et al. (Krug et al, 1976) as

$$\Delta G^0_{sol} = -RT \times intercept \qquad \text{…..…..} (6)$$

In which the intercept used is that obtained in plots of lnx_B as a function of $(1/T - 1/Tmean)$. The standard molar entropy change ΔS^0_{soln} is obtained from

$$\Delta S^0_{Sol} = \frac{\Delta H^0_{Sol} - \Delta H^0_{Sol}}{T_{mean}} \qquad \text{…..……} (7)$$

Both ΔG^0_{soln} and ΔS^0_{soln} pertain to the mean temperature T_{mean} = 302.92 K.

The results are shown in Table 5, together with $\%\zeta H$ and $\%\zeta TS$. It is worthy to note that relative contribution of enthalpy $\%\zeta H$ and $\%\zeta TS$ which are defined as

$$\%\zeta_H = \frac{\Delta H^0_{Sol}}{|\Delta H^0_{Sol}| + |T\Delta S^0_{Sol}|} X100 \qquad \text{……..} (8)$$

$$\%\zeta_{TS} = \frac{|T\Delta S^0_{Sol}|}{|\Delta H^0_{Sol}| + |T\Delta S^0_{Sol}|} X100 \qquad \text{……..} (9)$$

can be simply used to calculate the main contributors of enthalpy or entropy to ΔG^0_{soln} (Cui et al, 2013). The values of ΔH^0 and ΔS^0 for all solutions are positive indicating the solution process as endothermic. The contribution of enthalpy is more as compared to entropy for all solutions.

Table 4. Slope(m) and Intercept(c) of the lnx_B vs. 10000($1/T - 1/T_{mean}$) Plot along with R^2

Water + 1-Propanol+Catechol			
x_c^0	m	c	R^2
0.0000	-5032	-1.982	0.992
0.1000	-2054	-1.432	0.999
0.2001	-1582	-1.251	0.996
0.2999	-1261	-1.143	0.997
0.4001	-1143	-1.078	0.995
0.5000	-965.1	-1.042	0.975
0.6000	-1048	-1.024	0.995
0.6998	-946.5	-0.974	0.993
0.8002	-903.4	-0.957	0.994
0.8999	-873.4	-0.946	0.993
1.0000	-970.9	-0.962	0.977

Density values are used to calculate excess molar functions (Pawar R.R. and Aher C. S., 2018).

CONCLUSIONS

The solubility of catechol is more in 1-propanol than in water and increases with increase in mole fraction of 1-propanol. ΔH^0_{soln} values are higher in water than water+1-propanol mixture and lowest in 1-propanol indicates the solubility trend in various solvents. Density of solution is depends on solubility of solute and solvent system both.

Solubility data and Thermodynamic functions including ΔH^0_{soln}, ΔG^0_{soln}, and ΔS^0_{soln} of catechol in water, 1-propanol and their mixture are more useful in field of physical chemistry and chemical engineering calculations involving fluid flow, heat and mass transfer, pharmaceutical industry, agriculture, biology, medicine. Solubility data is required for selection of proper solvent and design an optimized crystallization process.

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Corresponding author: Dr. Chandrakant Shivaji Aher, M. S. G. College, Malegaon Camp, Malegaon, Dist. Nashik, Maharashtra, India.
Email: chandsaher1980@rediffmail.com