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Physicochemical properties of some pyrimidine derivatives in some organic solvents

Abstract

Some physicochemical parameters such as density, refractive index and conductance of some newly synthesized pyrimidine derivatives have been measured in N, N-dimethyl formamide, chloroform and methanol at 308.15K. It is observed that these studied parameters depend on the solvent and structure of compounds, which may be due to different type of interactions.

Keywords: density, refractive index, conductance, methanol, N, N-dimethyl formamide, chloroform

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Shipra Baluja, Asmita Hirapara, Divyata Lava
Department of Chemistry, Saurashtra University, India

Correspondence: Shipra Baluja, Department of Chemistry, Saurashtra University, Rajkot-360005 (India), Tel +91-9687692918, Email Shipra_baluja@rediffmail.com

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Introduction

Heterocyclic compounds play an immense role in many biochemical processes[1] and numerous heterocyclic compounds are biosynthesized by plants and animals, which are also associated to significant biological properties. Nitrogen containing heterocyclic compounds are known to play an essential role in many living systems. The nucleic acid bases are the derivatives of pyrimidine and purine,[2] found in RNA and DNA in the form of uracil, thymine, cytosine, adenine and guanine. These nitrogen containing heterocycles are synthetically challenging models for a number of physiologically active natural products.[3]

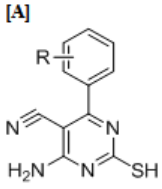
Pyrimidines are always an attraction point for researchers due to their pharmacological usages. These compounds are known to possess wide spectrum of biological activities such as anti-tubercular, anti-HIV, anti-microbial, anti-analgesic, anti-inflammatory and anti-malarial, antidepressant, anticonvulsant, antioxidant, anticancer, antifungal, etc.[4–16].

Thus, due to these biologically activity of pyrimidines, in the present paper, different pyrimidines compounds i.e., tetrahydropyrimidines and 2, 4-disubstituted pyrimidines have been synthesized. Some physicochemical properties such as density, refractive index and conductance of solutions of these synthesized compounds have been studied in different solvents at 308.15K.

Experimental

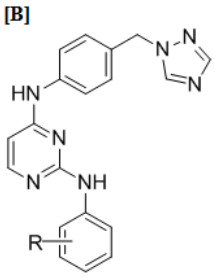
Some new tetrahydropyrimidines and 2, 4-disubstituted pyrimidines compounds have been synthesized. The general structures and substitutions in different compounds are given in Figure 1.

[A]



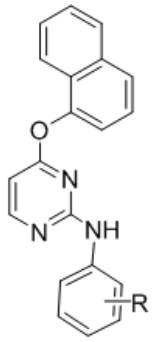
Where R is : SNS-1: 4-OH, 3-OCH_3-C_6H_4; SNS-2: 4-OCH_3-C_6H_4; SNS-3: 4-OH-C_6H_4; SNS-4: 4-Cl-C_6H_4; SNS-5: 3-Cl-C_6H_4; SNS-6: 4-F-C_6H_4; SNS-7: 3-NO_2-C_6H_4; SNS-8: -C_6H_5; SNS-9: C_4H_3O; SNS-10: -CH=CH-C_6H_5;

[B]



Where R is: SDN-1: 4-Cl; SDN-2: 4-CH_3; SDN-3: 4-F; SDN-4: 3-CF_3; SDN-5: 3-Cl, 4-F;

[C]



Where R is: SDO-1: 4-Cl; SDO-2: 4-CH_3; SDO-3: 4-F; SDO-4: 3-CF_3; SDO-5: 3-Cl, 4-F.

Figure 1 General structure of synthesized different pyrimidine derivatives: [A] tetrahydropyrimidines (SNS series); [B] 2, 4-disubstituted pyrimidines (SDN series) and [C] 2, 4-disubstituted pyrimidines (SDO series)

Physicochemical studies

The solvents DMF, chloroform and methanol used for physicochemical studies were purified by fractionally distillation by the reported method.[17] For each compound, a series of solutions of different concentrations were prepared in these solvents. The choice of different solvents for different compounds is due to solubility problem.

The density and refractive index of pure solvents and solutions

were measured by using pycnometer and Abbe refractometer respectively at 308.15K. The desired temperature was maintained by circulating water through jacket around the prisms of refractometer from an electronically controlled thermostatic water bath (NOVA NV-8550 E). The uncertainty of temperature was ±0.1°C.

The conductance of each solution was measured by using Elico Conductivity Meter (Model No. CM 180) at 308.15K. The measured conductance was corrected by subtracting the conductance of pure solvent.

Results and discussion

Density and refractive index

Table 1 shows the experimental values of densities and refractive index for all the studied solutions. Using experimental density of solution, density of each compound was calculated using the following relation:

$$\frac{1}{\rho_{12}} = \frac{g_1}{\rho_1} + \frac{g_2}{\rho_2} \quad (1)$$

Table 1 The density (ρ_{12}) and refractive index (n) of synthesized compounds at 308.15K

Conc. M	ρ_{12} g.cm^{-3}	n	ρ_{12} g.cm^{-3}	N
Tetrahydropyrimidines				
	DMF		**Chloroform**	
SNS-1				
0.00	0.9338	1.4239	1.4713	1.4397
0.01	0.9456	1.4231	1.4715	1.4402
0.02	0.9465	1.4239	1.4718	1.4410
0.04	0.9483	1.4247	1.4721	1.4421
0.06	0.9500	1.4255	1.4726	1.4433
0.08	0.9516	1.4265	1.4731	1.4448
0.10	0.9535	1.4273	1.4737	1.4458
SNS-2				
0.01	0.9448	1.4223	1.4717	1.4399
0.02	0.9452	1.4229	1.4724	1.4404
0.04	0.9461	1.4238	1.4736	1.4414
0.06	0.9470	1.4248	1.4749	1.4423
0.08	0.9479	1.4259	1.4761	1.4433
0.10	0.9489	1.4268	1.4774	1.4443
SNS-3				
0.01	0.9486	1.4212	1.4714	1.4400
0.02	0.9489	1.4228	1.4718	1.4406
0.04	0.9495	1.4230	1.4727	1.4417
0.06	0.9501	1.4242	1.4736	1.4428
0.08	0.9507	1.4252	1.4745	1.4440
0.10	0.9513	1.4263	1.4754	1.4450
SNS-4				
0.01	0.9494	1.4219	1.4749	1.4415

Table Continued....

0.02	0.9503	1.4223	1.4753	1.4416
0.04	0.9520	1.4231	1.4761	1.4420
0.06	0.9538	1.4239	1.4768	1.4423
0.08	0.9555	1.4250	1.4776	1.4425
0.10	0.9573	1.4255	1.4784	1.4428
SNS-5				
0.01	0.9494	1.4203	1.4720	1.4409
0.02	0.9503	1.4208	1.4723	1.4410
0.04	0.9520	1.4217	1.4730	1.4413
0.06	0.9538	1.4226	1.4736	1.4416
0.08	0.9556	1.4235	1.4743	1.4418
0.10	0.9573	1.4244	1.4750	1.4421
SNS-6				
0.01	0.9454	1.4211	1.4747	1.4412
0.02	0.9458	1.4215	1.4752	1.4414
0.04	0.9467	1.4222	1.4762	1.4418
0.06	0.9476	1.4230	1.4772	1.4425
0.08	0.9484	1.4237	1.4782	1.4426
0.10	0.9494	1.4244	1.4792	1.4430
SNS-7				
0.01	0.9529	1.4191	1.4800	1.4408
0.02	0.9530	1.4200	1.4801	1.4412
0.04	0.9531	1.4217	1.4803	1.4420
0.06	0.9535	1.4234	1.4805	1.4426
0.08	0.9537	1.4252	1.4807	1.4433
0.10	0.9540	1.4269	1.4809	1.4440
SNS-8				
0.01	0.9506	1.4225	1.4735	1.4408
0.02	0.9517	1.4228	1.4737	1.4411
0.04	0.9528	1.4234	1.4741	1.4416
0.06	0.9531	1.4239	1.4744	1.4421
0.08	0.9547	1.4245	1.4748	1.4426
0.10	0.9551	1.4251	1.4751	1.4431
SNS-9				
0.01	0.9424	1.4164	1.4809	1.4397
0.02	0.9429	1.4175	1.4813	1.4400
0.04	0.9440	1.4195	1.4820	1.4406
0.06	0.9451	1.4214	1.4827	1.4412
0.08	0.9462	1.4234	1.4834	1.4418
0.10	0.9473	1.4253	1.4741	1.4424
SNS-10				
0.01	0.9562	1.4233	1.4746	1.4396
0.02	0.9565	1.4238	1.4751	1.4398
0.04	0.9571	1.4244	1.4763	1.4399
0.06	0.9576	1.4251	1.4775	1.4401
0.08	0.9581	1.4257	1.4787	1.4402

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Table Continued....

0.10	0.9587	1.4262	1.4798	1.4404
2, 4-disubstituted pyrimidines				
	DMF		**Methanol**	
SDN-1				
0.00	0.9338	1.4239	0.7770	1.3250
0.01	0.9432	1.4245	0.7794	1.3260
0.02	0.9446	1.4255	0.7812	1.3265
0.04	0.9468	1.4270	0.7839	1.3295
0.06	0.9484	1.4285	0.7879	1.3310
0.08	0.9497	1.4295	0.7892	1.3325
0.10	0.9516	1.4310	0.7909	1.3330
SDN-2				
0.01	0.9430	1.4240	0.7816	1.3265
0.02	0.9441	1.4245	0.7839	1.3280
0.04	0.9462	1.4260	0.7880	1.3300
0.06	0.9479	1.4270	0.7915	1.3315
0.08	0.9491	1.4285	0.7948	1.3330
0.10	0.9504	1.4300	0.7997	1.3345
SDN-3				
0.01	0.9428	1.4250	0.7804	1.3280
0.02	0.9438	1.4260	0.7819	1.3295
0.04	0.9455	1.4275	0.7837	1.3315
0.06	0.9474	1.4295	0.7869	1.3330
0.08	0.9489	1.4310	0.7883	1.3345
0.10	0.9501	1.4320	0.7893	1.3360
SDN-4				
0.01	0.9434	1.4250	0.7830	1.3265
0.02	0.9447	1.4265	0.7851	1.3285
0.04	0.9474	1.4285	0.7883	1.3310
0.06	0.9506	1.4300	0.7907	1.3325
0.08	0.9520	1.4315	0.7932	1.3345
0.10	0.9541	1.4325	0.7969	1.3380
SDN-5				
0.01	0.9432	1.4255	0.7798	1.3265
0.02	0.9445	1.4270	0.7821	1.3280
0.04	0.9470	1.4285	0.7860	1.3295
0.06	0.9492	1.4300	0.7889	1.3330
0.08	0.9512	1.4320	0.7921	1.3360
0.10	0.9525	1.4315	0.7958	1.3405
	DMF		**Methanol**	
SDO-1				
0.01	0.9425	1.4245	0.7791	1.3265
0.02	0.9440	1.4260	0.7802	1.3270
0.04	0.9467	1.4275	0.7824	1.3275
0.06	0.9490	1.4280	0.7847	1.3280
0.08	0.9517	1.4300	0.7868	1.3290

Table Continued....

0.10	0.9529	1.4320	0.7894	1.3305
SDO-2				
0.01	0.9422	1.4240	0.7793	1.3260
0.02	0.9434	1.4245	0.7809	1.3270
0.04	0.9449	1.4255	0.7831	1.3275
0.06	0.9488	1.4265	0.7857	1.3285
0.08	0.9502	1.4280	0.7872	1.3294
0.10	0.9513	1.4295	0.7912	1.3315
SDO-3				
0.01	0.9428	1.4240	0.7795	1.3260
0.02	0.9447	1.4245	0.7809	1.3275
0.04	0.9461	1.4255	0.7829	1.3290
0.06	0.9496	1.4260	0.7855	1.3305
0.08	0.9520	1.4270	0.7876	1.3315
0.10	0.9535	1.4281	0.7914	1.3335
SDO-4				
0.01	0.9429	1.4240	0.7801	1.3265
0.02	0.9452	1.4245	0.7824	1.3260
0.04	0.9471	1.4255	0.7864	1.3270
0.06	0.9489	1.4270	0.7898	1.3280
0.08	0.9507	1.4285	0.7923	1.3295
0.10	0.9530	1.4295	0.7950	1.3330
SDO-5				
0.01	0.9431	1.4245	0.7797	1.3260
0.02	0.9449	1.4265	0.7814	1.3275
0.04	0.9468	1.4290	0.7844	1.3285
0.06	0.9495	1.4315	0.7869	1.3295
0.08	0.9520	1.4325	0.7885	1.3305
0.10	0.9540	1.4340	0.7923	1.3315

where ρ_{12} is the density of solution and ρ_1 and ρ_2 are the densities of solvent and solute respectively. g_1 and $g_2$are the weight fractions of solvent and solute.

The evaluated densities of all the compounds are listed in Table 2 along with the theoretical densities, which were calculated using the following equation:[18]

$$\rho = KM \Big/ N_A \sum \Delta V_i \qquad (2)$$

where ρ is the density of the compound, K is packing fraction (0.599), M is the molecular weight of the compound, N_A is the Avogadro's number and ΔV_i is the volume increment of the atoms and atomic groups present in the compound.

Comparison of densities values showed that theoretical density values are different from those evaluated from experimental data. Further, for the same compound, density in the two solvents is different. This suggests that solvent plays an important role. In solutions, compounds interact differently depending upon their substitution, structure and nature of solvent. These molecular interactions affect volume, which causes change in density.

Further, the molar refraction of a pure liquid $(MRD)_1$ were calculated by the following equation:

$$\left(MRD\right)_1 = \left[\frac{n^2-1}{n^2+1}\right]\frac{M}{\rho} \quad (3)$$

where n, M and ρ are refractive index, molecular weight and density pure liquid respectively.

Table 2 Experimental and theoretical densities of compounds at 308.15K

Compounds	Experimental density g.cm^{-3}		Theoretical density g.cm^{-3}
	DMF	**Chloroform**	
SNS-1	1.5175	1.6234	1.2960
SNS-2	1.2270	1.9380	1.2624
SNS-3	1.2870	1.7825	1.3163
SNS-4	1.7953	1.8692	1.3565
SNS-5	1.7699	1.6978	1.3565
SNS-6	1.2610	2.0121	1.3351
SNS-7	1.2438	1.8519	1.3664
SNS-8	1.2315	1.6892	1.2787
SNS-9	1.2642	2.4213	1.5300
SNS-10	1.5974	2.0661	1.3877
	DMF	**Methanol**	
SDN-1	1.2804	1.2484	1.3612
SDN-2	1.2531	1.9417	1.2766
SDN-3	1.3405	1.1628	1.3485
SDN-4	1.3605	1.3680	1.6028
SDN-5	1.3021	1.4599	1.4420
SDO-1	1.4368	1.1919	1.1947
SDO-2	1.3870	1.3123	1.1177
SDO-3	1.4306	1.7007	1.1787
SDO-4	1.3228	1.2063	1.3514
SDO-5	1.4225	1.2887	1.2192

For solutions, the following equation was used to determining molar refraction:

$$\left(MRD\right)_{12} = \left[\frac{n_{12}^2-1}{n_{12}^2+1}\right]\left[\frac{X_1M_1 + X_2M_2}{\rho_{12}}\right] \quad (4)$$

where n_{12} and ρ_{12} are refractive index and density of solution respectively. X_1 and X_2 are the mole fractions and M_1 and M_2 are the molecular weight of the solvent and solute respectively.

From the values of the molar refraction of solution and pure solvent, molar refraction of solid compounds were determined by following equation:

$$\left(MRD\right)_{12} = X_1\left(MRD\right)_1 + X_2\left(MRD\right)_2 \quad (5)$$

From the density and molar refraction data, the refractive indexes of all the compounds were calculated from eq. (5). The molar refraction $(MRD)_2$ and refractive index of all the compounds are reported in Table 3 for 0.1M solution.

It is evident from Table 3 that both $(MRD)_2$ and refractive index of compounds are different in each solvent. This again proves that in different solvents, intermolecular interactions are different, which affect these parameters. In some solvents, there may be interaction between solute and solvent molecules where as in others breakage of bonds may take place. As refractive index and molar refraction depends upon not only atomic refraction but also upon single, double or triple bonds, the type of interactions taking place in solution affects these parameters. Further, bond polarity also causes change in molar refraction. Thus, type of solvent affects the refractive index and molar refraction of a solute.

Table 3 Molar refraction $(MRD)_2$ and refractive index (n) of 0.1M solutions of compounds at 308.15K

Compounds	(MRD_2)	n	(MRD_2)	N
Solvents				
	DMF		**Chloroform**	
SNS-1	121.62	1.7680	76.53	1.4703
SNS-2	127.01	1.6448	59.26	1.4469
SNS-3	114.30	1.5263	64.01	1.3921
SNS-4	99.00	1.7553	50.46	1.3539
SNS-5	94.42	1.7361	53.75	1.3576
SNS-6	109.83	1.5803	47.02	1.3722
SNS-7	119.41	1.5820	54.05	1.3677
SNS-8	104.12	1.5317	51.63	1.3419
SNS-9	112.69	1.6026	30.06	1.2799
SNS-10	96.77	1.6999	33.79	1.2784
	DMF		**Methanol**	
SDN-1	116.23	1.7175	107.01	1.6251
SDN-2	108.67	1.6872	87.16	1.9230
SDN-3	121.28	1.8583	124.15	1.7308
SDN-4	126.43	1.7764	128.42	1.7989
SDN-5	121.29	1.7296	141.56	2.0683
SDO-1	109.87	1.8569	88.87	1.5211
SDO-2	95.38	1.7731	84.56	1.5932
SDO-3	82.26	1.6053	86.98	1.8493
SDO-4	122.39	1.9435	106.60	1.5894
SDO-5	105.28	1.6510	91.59	1.5586

Conductance

The measured conductance (k) of each solution after correction are given in Table 4. It is observed that for all the studied compounds, conductance increases with concentration in all the solvents. The conductance measurement of two tetrahydropyrimidine compounds SNS-1 and SNS-3 cannot be done as these compounds had very less solubility in chloroform. For both tetrahydropyrimidines 2, 4-disubstituted pyrimidine compounds, conductance is lower in DMF than that in chloroform and methanol respectively.

From corrected conductance, specific conductance (κ) and equivalent conductance (λ_c) are calculated using the following equations:

$$\kappa = k\theta \quad (6)$$

$$\lambda_c = 1000\frac{\kappa}{C} \quad (7)$$

where θ is the cell constant (0.96cm^{-1}) and c is the concentration (g.equi./lit.) of solution.

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Table 4 The conductance (k) of synthesized compounds in different solvents at 308.15K

Conc. M	$k \cdot 10^4$ mho									
Tetrahydropyrimidines										
DMF										
	SNS -1	**SNS -2**	**SNS -3**	**SNS -4**	**SNS -5**	**SNS -6**	**SNS -7**	**SNS -8**	**SNS -9**	**SNS -10**
0.000	0.2800	0.2800	0.2800	0.2800	0.2800	0.2800	0.2800	0.2800	0.2800	0.2800
0.001	0.0187	0.0174	0.0017	0.0089	0.0050	0.0017	0.0013	0.0122	0.0030	0.0209
0.002	0.0370	0.0346	0.0034	0.0169	0.0094	0.0028	0.0021	0.0238	0.0059	0.0414
0.004	0.0728	0.0684	0.0064	0.0326	0.0170	0.0057	0.0040	0.0454	0.0115	0.0804
0.006	0.1062	0.0988	0.0094	0.0463	0.0243	0.0077	0.0053	0.0660	0.0165	0.1140
0.008	0.1336	0.1284	0.0111	0.0580	0.0295	0.0088	0.0051	0.0843	0.0184	0.1424
0.010	0.1420	0.1526	0.0075	0.0675	0.0306	0.0100	0.0043	0.1000	0.0190	0.1550
0.020	0.1979	0.2453	0.0279	0.1121	0.0494	0.0291	0.0106	0.1421	0.0352	0.2467
0.040	0.2246	0.3684	0.0470	0.2020	0.0730	0.0684	0.0198	0.1876	0.0620	0.3206
0.060	0.2495	0.4080	0.1009	0.2735	0.0726	0.0996	0.0178	0.2331	0.0720	0.3947
0.080	0.2738	0.3449	0.1258	0.3459	0.0746	0.1299	0.0176	0.2779	0.0756	0.4689
0.100	0.2992	0.2707	0.1595	0.4185	0.0709	0.1586	0.0107	0.3241	0.0783	0.5431
Chloroform										
0.000	0.084	0.084	0.084	0.084	0.084	0.084	0.084	0.084	0.084	0.084
0.001	-	0.0890	-	0.0890	0.0850	0.1000	0.1050	0.1038	0.1246	0.1187
0.002	-	0.1740	-	0.1558	0.1335	0.1880	0.1860	0.2003	0.2373	0.2225
0.004	-	0.3400	-	0.2967	0.2373	0.3560	0.3227	0.3560	0.4450	0.4050
0.006	-	0.4980	-	0.3900	0.3120	0.4680	0.4160	0.4800	0.6000	0.5680
0.008	-	0.6240	-	0.5200	0.3740	0.5280	0.5020	0.5512	0.7390	0.6760
0.010	-	0.6400	-	0.4450	0.4020	0.5500	0.5120	0.5680	0.8460	0.7400
0.020	-	0.8900	-	0.7000	0.6230	0.8900	0.7120	1.0680	1.2460	1.1570
0.040	-	0.9790	-	0.8010	0.6230	0.8900	0.8010	1.2460	1.7350	1.6460
0.060	-	0.9790	-	0.8900	0.7120	0.9790	0.8900	1.3350	1.9350	1.8000
0.080	-	1.0680	-	0.8900	0.7120	0.9790	0.9790	1.4240	2.0640	1.6800
0.100	-	1.0680	-	0.9790	0.8010	0.9790	1.1570	1.6020	1.9900	1.5130
2,4-Disubstituted pyrimidines										
DMF										
	SDN-1	**SDN -2**	**SDN -3**	**SDN -4**	**SDN -5**	**SDO -1**	**SDO-2**	**SDO-3**	**SDO-4**	**SDO-5**
0.000	0.2800	0.2800	0.2800	0.2800	0.2800	0.2800	0.2800	0.2800	0.2800	0.2800
0.001	0.0735	0.2037	0.1200	0.1851	0.0828	0.0642	0.1107	0.2967	0.1851	0.2595
0.002	0.2130	0.3525	0.2874	0.3060	0.2316	0.2781	0.3339	0.5757	0.4827	0.5850
0.004	0.4362	0.6780	0.5943	0.5385	0.4362	0.6687	0.6780	1.0221	1.0128	1.1988
0.006	0.6036	0.9105	0.8361	0.7803	0.5943	1.0221	0.9849	1.4313	1.3941	1.6452
0.008	0.7802	1.1058	1.0593	0.9662	0.7524	1.3569	1.2360	1.8218	1.8405	2.0544
0.010	0.8547	1.3197	1.4127	1.1523	0.9291	1.7010	1.4871	2.2497	2.2404	2.3241
0.020	1.3940	2.1938	2.0916	1.5986	1.4778	2.8262	2.3612	3.6726	4.3700	3.9702
0.040	2.2684	3.0868	3.3284	2.4076	2.4544	3.9700	4.1656	6.4440	6.8532	5.4116
0.060	2.6496	3.6540	3.9330	3.1890	3.2262	5.3928	5.2440	8.1828	7.6530	6.3138
0.080	3.0216	4.2960	4.1656	3.7008	4.0072	6.3512	5.8952	9.2896	8.0992	7.2064
0.100	3.2630	4.4540	4.2310	4.1840	4.2030	6.8900	6.4250	9.5220	8.6020	8.3500
Methanol										

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Table Continued....

0.000	0.0400	0.0400	0.0400	0.0400	0.0400	0.0400	0.0400	0.0400	0.0400	0.0400
0.001	0.0558	0.4929	0.0837	0.0651	0.0372	0.0558	0.0465	0.8928	0.9951	0.7254
0.002	0.2511	0.9021	0.4278	0.6045	0.5115	0.2465	0.5673	1.9158	1.9902	1.7112
0.004	0.7719	1.7949	1.2369	1.5066	1.4415	0.8928	1.5252	3.8967	3.7851	3.5247
0.006	1.2927	2.5854	1.9065	2.4924	2.2599	1.4880	2.5017	5.7195	5.7102	5.0406
0.008	1.8414	3.3759	2.7528	3.3108	3.1713	2.0181	3.3945	7.6818	7.3842	6.0450
0.010	2.2320	3.9339	3.3108	4.1943	4.3617	2.5017	4.6128	9.0954	8.7234	7.6167
0.020	4.0827	7.5516	6.2589	8.0538	7.8492	4.0827	8.5002	15.9774	15.1404	12.6294
0.040	6.5100	13.0014	11.2344	14.0244	13.0014	10.0347	13.9314	25.5564	24.9984	21.0924
0.060	9.6813	19.1394	15.9774	19.2324	17.7444	14.1174	19.3254	34.2984	33.8334	27.8814
0.080	12.0807	23.0454	22.5804	23.7894	21.8364	18.0234	23.8824	42.6684	40.5294	33.8334
0.100	15.3264	27.9744	25.8354	25.9284	25.7424	24.4404	28.9044	49.2714	45.6444	38.3904

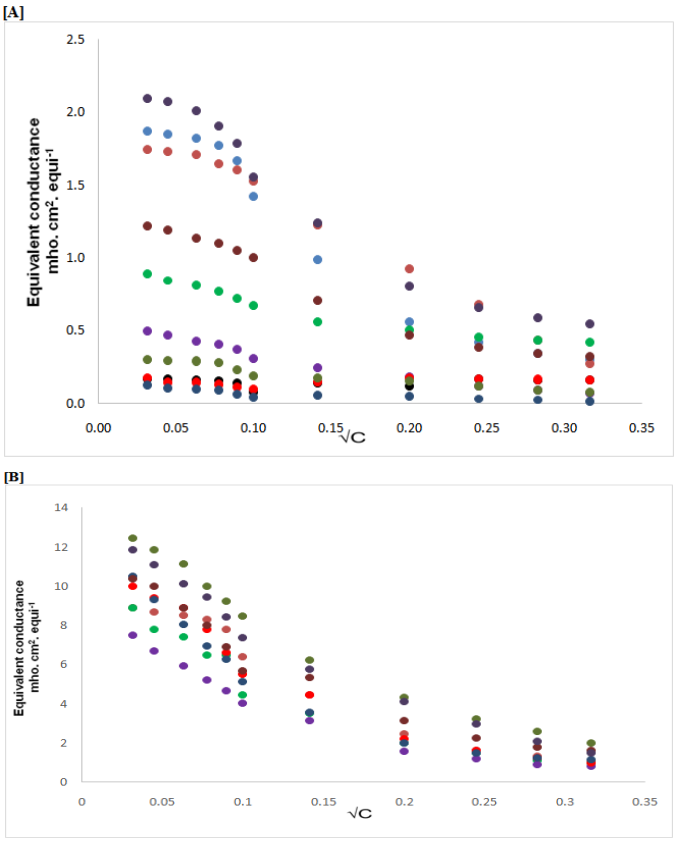

Figure 2 The variation of equivalent conductance with √C for tetrahydropyrimidines in [A] DMF and [B] chloroform at 308.15K.
●: SNS-1; ●: SNS-2; ●: SNS-3; ●: SNS-4; ●: SNS-5; ●: SNS-6; ●: SNS-7 ●: SNS-8; ●: SNS-9; ●: SNS-10.

The equivalent conductance (λ_c) is plotted against √C for all compounds as shown in Figure 2-4. For tetrahydropyrimidine compounds, in DMF, equivalent conductance increases with concentration in both the solvents. At higher concentrations, the variation of equivalent conductance for different compounds is very less. Further, in DMF, equivalent conductance for tetrahydropyrimidine compounds are much lower than those in chloroform. It is obvious from Figure 2 that in DMF, most of tetrahydropyrimidine compounds behave as weak electrolytes whereas in chloroform, these compounds exhibited electrolytic behavior. For 2, 4-disubstituted pyrimidine compounds (both SDN and SDO compounds) also, equivalent conductance is less in DMF solutions than those in methanol solutions. Figure 3 shows that in DMF, SDN-2 and SDN-4 showed electrolytic behavior whereas for SDN-1, SDN-3 and SDN-5 compounds, equivalent conductance decreases at lower concentration. In methanol also, except SDN-2, for other four compounds also equivalent conductance decreases at lower concentration. Similar behavior was also observed for SDO compounds in both DMF and methanol solutions except SDO-3 in DMF (Figure 4). This typical behavior may be due to interactions within the molecule thereby causing constriction within the molecule or due to association between solute with solvent molecules. Similar behavior was observed by Singh et al.[19,20]

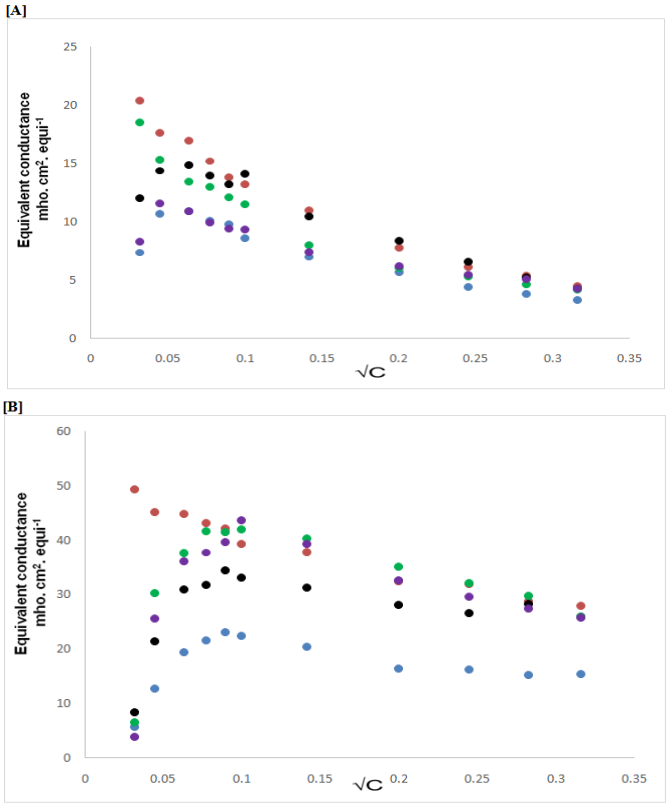

Figure 3 The variation of equivalent conductance with √C for 2, 4-disubstituted pyrimidines (SDN series) in [A] DMF and [B] Methanol at 308.15K.
●: SDN-1; ●: SDN-2; ●: SDN-3; ●: SDN-4; ●: SDN-5.

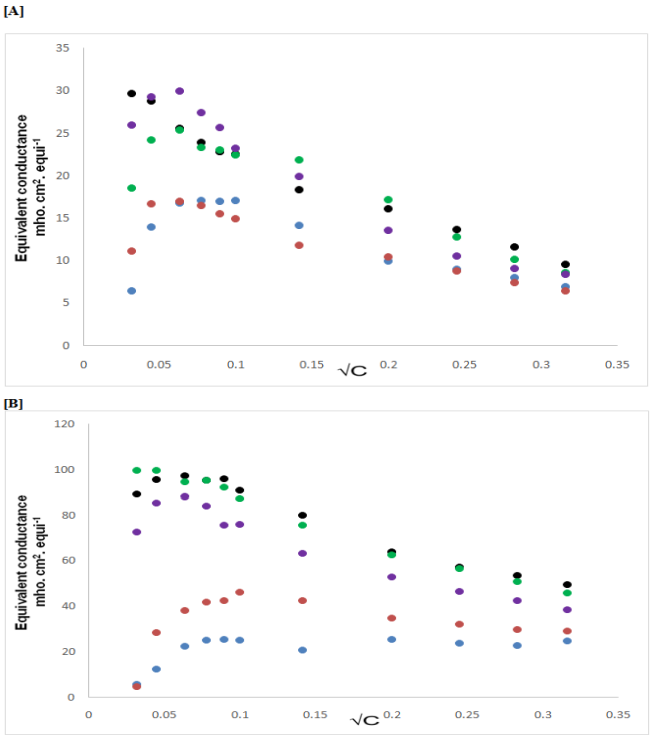

Figure 4 The variation of equivalent conductance with √C for 2, 4-disubstituted pyrimidines (SDO series) in [A] DMF and [B] Methanol at 308.15K.

●: SDO-1; ●: SDO-2; ●: SDO-3; ●: SDO-4; ●: SDO-5.

Conclusion

It is observed that physicochemical parameters of compounds in solution depends not only on the structure and substitution of the compound but also on the nature of solvent in which it is dissolved. The molecular interactions occurring in the solution affect volume which in turn causes a small change in density and refractive index. Depending upon the nature of solvent, the conductance i.e., electrolytic behavior of compounds also changes.

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None.

Conflict of interest

The author declares that there is no conflict of interest.

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