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Interaction of Chloropyriphos with Aqueous Organic Solvents as O-Xylene and P-Xylene

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Abstract

Chloropyriphos is a crystalline organophosphate insecticide that inhibits acetylcholinesterase and is used to control insect pests. Ultrasonic velocity, Density and Viscosity measurements have been used to calculate Ultrasound velocity (V), Density (ρ), Excess viscosity (η), Specific acoustic impedance (Z), Rao's constant (R), Shear's relaxation time (τ_s), Apparent molal adiabatic compressibility (Φ_k) Isentropic compressibility (β_s), Intermolecular free length (L_f), and Excess values (A^E) of solutions of pesticides- Chloropyriphos in aqueous organic solvents such as O-xylene and P-xylene. In each case, Ultrasound velocity decreases and isentropic compressibility (β_s), intermolecular free length (L_f), density (ρ) and viscosity increases with the increases in molar concentration of Chloropyriphos. The results have been interpreted in terms of ion-solvent interaction on the basis of acoustic properties. As usual apparent molal adiabatic compressibility (Φ_k) has been found to be negative in both cases.

Keywords: Chloropyriphos, O-xylene, P-xylene, Interferometric technique and Acoustic properties.

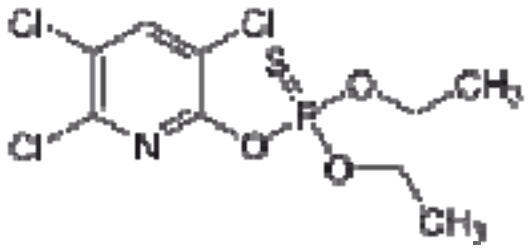
Introduction

Chloropyriphos is a crystalline organophosphate insecticide that inhibits acetylcholinesterase and is used to control insect pests. IUPAC name of Chloropyriphos is O,O-diethyl O-3,5,6-trichloro-2-pyridyl phosphorothioate and manufactured by reacting 3,5,6-trichloro-2-pyridinol with diethylthiophosphoryl chloride[1]. Pesticides are chemicals and biological material that are used by mean to reduce pest organisms[2]. The greatest use of pesticides in any country is for

agriculture and forest pest control[3].Pesticides are vital for increasing the agriculture yield by reducing crop losses and insuring optimum utilization of fertilizers and seeds(4). Present work covers and extensive survey of physico- chemical and solvolytic studies of some pesticides-Chloropyriphos in aqueous organic solvents such as o-xylene and p-xylene systems studied at various temperature (25^0C, 30^0C and 35^{0C})[5]. Lagemann and Dunbar was the first point out the sound velocity approach for qualitative determination of the degree of association in liquids, to study the behaviour of binary liquid mixtures by measuring the sound velocity and related properties[6].

The compressibility of the dilute aqueous solution of pesticides increases with increasing concentration of the dissolved ions with water molecules [7-8]. Present work is reporting the finding of a study of a ultrasound velocity, density and viscosity measurement have been used to calculate isentropic compressibility (β_s), intermolecular free length (L_f), molar volume (M_V), Rao's constant (R) , apparent molar adiabatic compressibility (Φ_k), shear's relaxation time(τ_s) of pesticides in solvent [9-10].

A continuous wave interferometric technique was employed for the measurement of ultrasonic velocity. The density and viscosity were determined using a vibrating densitometer. The experiment was repeated at least twice and results were reproducible with experimental error of 0.0002 kgm^{-3} and 0.0002 mPas respectively.



Chloropyriphos

Comutation of Different Physical Parameters

$$\beta_s = [1/(V^2 . \rho)]$$

$$Z = [V . \rho.10^3]$$

$$L_F = K \overline{\quad}$$

$$R = [- \cdot V^{1/3}]$$

$$R_A = (\rho/ \rho_o) . (v_o/v)^{1/3}$$

$$\Phi_k = 1000/(c.\rho_o) . (\rho_o . \beta_s - \beta_s o . \rho) + (\beta_s o . M/\rho_o)$$

$$\tau_s = 4/3 . \eta . \beta_s$$

$$S_n = n_1/n_2 [1- \beta_s/\beta_s o]$$

Where, V= ultrasound velocity, Z= specific acoustic impedance, β_s= isentropic compressibility, L_f = intermolecular free length, R= molar sound velocity, R_A= relative association, τ_s= shear's relaxation time, Φ_k= apparent molal compressibility and S_n=solvation number.

While ρ_o and $\beta_s o$ are density and compressibility of pure solvent and ρ_s and β_s are the density and compressibility of the solution respectively. C is the concentration in mole/litre of solute, M is the molecular weight of solute and n_1 and n_2 are the moles of solute and solvent respectively [11-17].

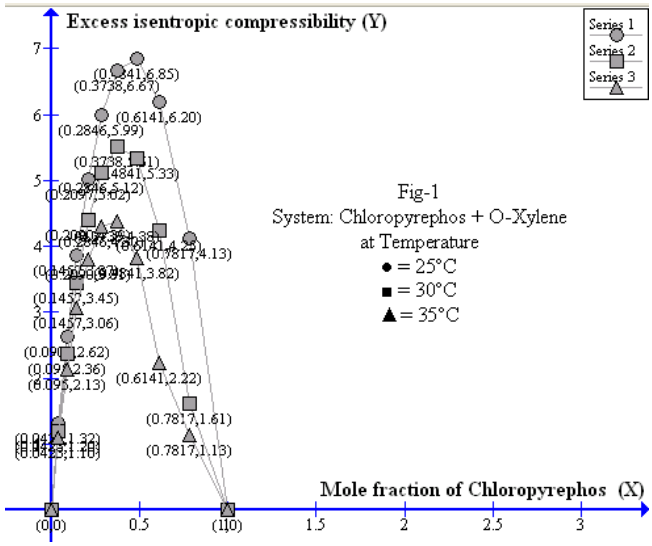


Figure 1: Excess isentropic compressibility v_s mole fraction of chloropyriphos + o-xylene.

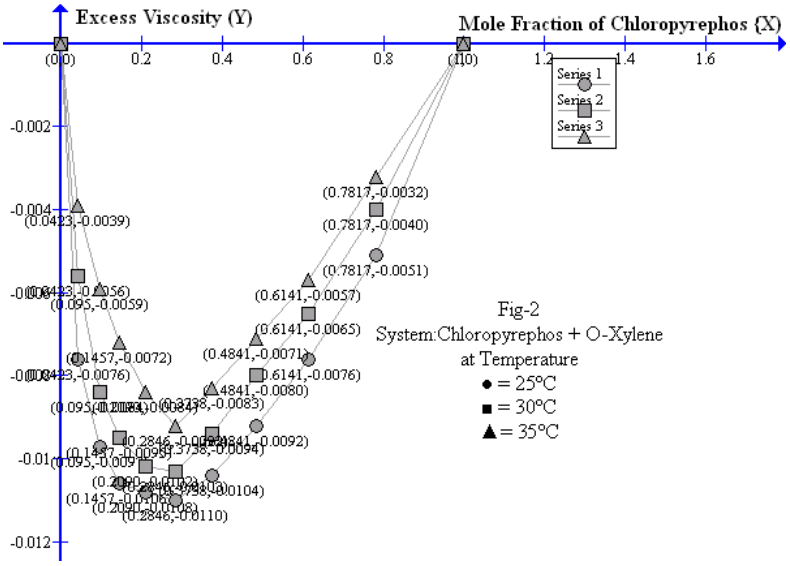


Figure 2: Lowering viscosity v_s mole fract- ion of chloropyriphos + o-xylene.

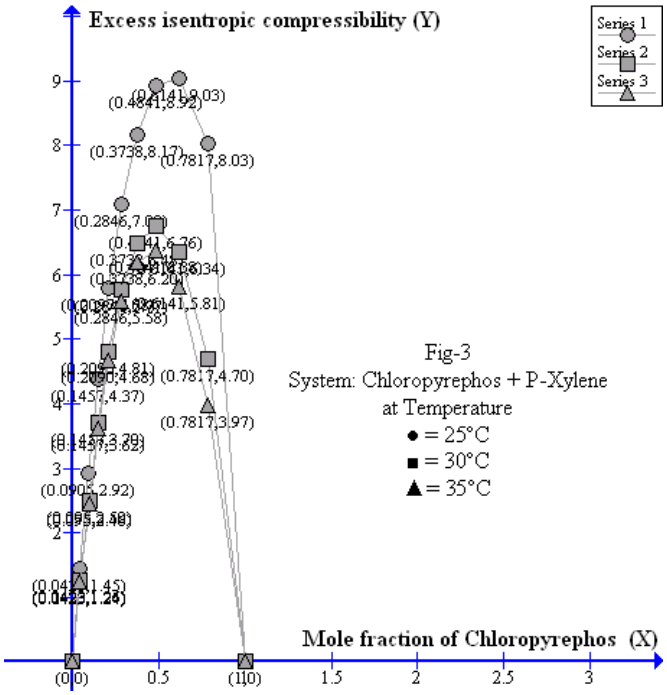


Figure 3: Excess isentropic compressibility v_s mole fraction of chloropyriphos + p-xylene.

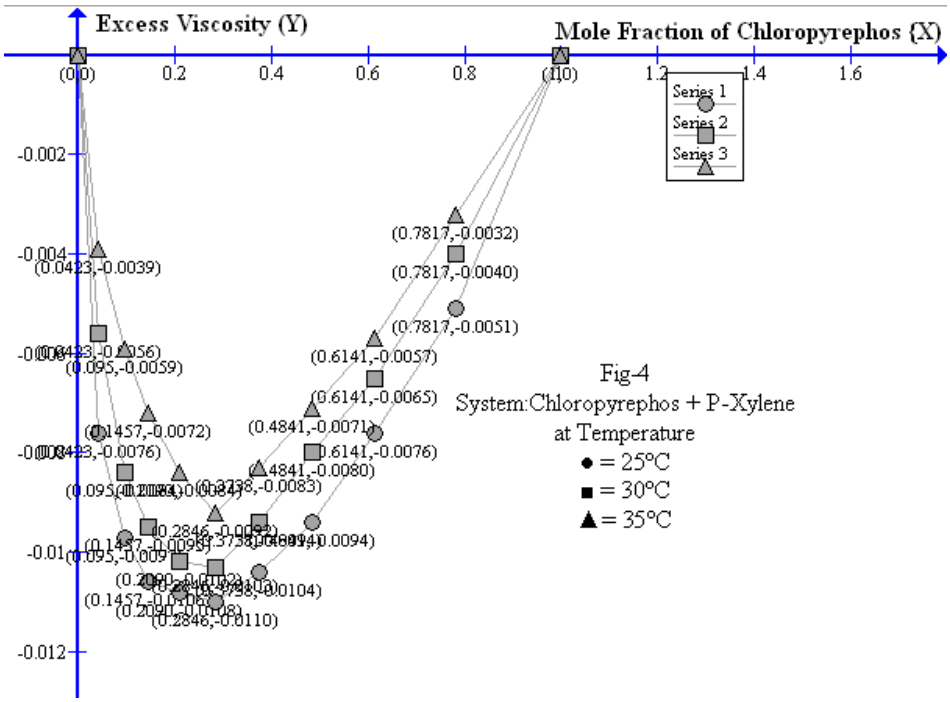


Figure 4: Lowering viscosity v_s mole fract-ion of chloropyriphos + p-xylene.

Table 1: Chloropyriphos + O-xylene at 25°C ± 0.05°C.

Conc(c)	V	ρ	Z	β_s	β_so	β_s- $\beta_{sO/C}$	L_f	η	η_{sp}	η- $\eta_{sp/C}$	M_V	R	τ_s
0.0000	1344	0.8865	1.1915	62.45	62.45	0.00	0.4986	0.7784	0.7784	0.0000	119.76	13.21	0.65
0.0423	1316	0.8909	1.1724	64.81	63.49	1.32	0.5079	0.7663	0.7739	-0.0076	122.31	13.40	0.66
0.0905	1288	0.8953	1.1531	87.33	64.70	2.62	0.5177	0.7589	0.7686	-0.0097	125.35	13.64	0.68
0.1457	1260	0.8997	1.1336	70.01	6614	3.87	0.5279	0.7518	0.7624	-0.0106	129.01	13.93	0.70
0.2097	1232	0.9041	1.1139	72.87	67.85	5.02	0.5386	0.7442	0.7550	-0.0108	133.48	14.31	0.72
0.2846	1204	0.9085	1.0938	75.93	69.94	5.99	0.5498	0.7349	0.7459	-0.0110	139.00	14.78	0.74
0.3738	1176	0.9129	1.0736	79.21	72.54	6.67	0.8615	0.7242	0.7346	-0.0104	145.99	15.41	0.76
0.4814	1148	0.9173	1.0531	82.72	75.87	6.85	0.5738	0.7109	0.7201	-0.0092	155.04	16.23	0.78
0.6141	1120	0.9217	1.0323	86.49	80.29	6.20	0.5868	0.6933	0.7009	-0.0076	167.17	17.36	0.80
0.7817	1092	0.9261	1.0113	90.55	86.42	4.13	0.6004	0.6692	0.6743	-0.0051	184.17	18.96	0.81
1.0000	1062	0.9282	0.9857	95.52	95.52	0.00	0.6167	0.6348	0.6348	0.0000	210.08	21.43	0.81

Table 2: Chloropyriphos + O-xylene at 30°C ± 0.05°C.

Conc.(c)	V	ρ	Z	β_s	β_so	β_s- $\beta_{s/C}$	L_f	η	η_{sp}	η- $\eta_{sp/C}$	M_V	R	τ_s
0.0000	1330	0.8715	1.1591	64.87	64.87	0.00	0.5126	0.7463	0.7463	0.0000	121.82	13.39	0.65
0.0423	1304	0.8756	1.1418	67.16	65.96	1.20	0.5116	0.7368	0.7424	-0.0056	124.45	13.59	0.66
0.0905	1278	0.8797	1.1243	69.60	67.24	2.36	0.5310	0.7295	0.7379	-0.0084	127.57	13.84	0.68
0.1457	1252	0.8838	1.1065	72.18	68.74	3.45	0.5407	0.7231	0.7326	-0.0095	131.33	14.15	0.70
0.2097	1226	0.8879	1.0886	74.93	70.54	4.39	0.5509	0.7161	0.7263	-0.0102	135.91	14.54	0.72
0.2846	1200	0.8920	1.0704	77.85	72.73	5.12	0.5616	0.7083	0.7185	-0.0103	141.58	15.04	0.74
0.3738	1174	0.8961	1.0520	80.97	75.46	5.51	0.5727	0.6994	0.7089	-0.0094	148.73	15.69	0.76
0.4814	1148	0.9002	1.0334	84.29	78.96	5.33	0.5843	0.6885	0.6965	-0.0080	157.99	16.54	0.77
0.6141	1122	0.9043	1.0146	87.84	83.59	4.25	0.5965	0.6737	0.6801	-0.0065	170.39	17.70	0.79
0.7817	1096	0.9084	0.9956	91.64	90.03	1.61	0.6093	0.6534	0.6574	-0.0040	187.76	19.35	0.80
1.0000	1050	0.9108	0.9563	99.59	99.59	0.00	0.6351	0.6236	0.6236	0.0000	214.10	21.76	0.83

Table 3: Chloropyriphos + O-xylene at 35°C ± 0.05°C.

Conc(c)	V	ρ	Z	β_s	β_so	β_s- $\beta_{s/C}$	L_f	η	η_{sp}	η- $\eta_{sp/C}$	M_V	R	τ_s
0.0000	1330	0.8715	1.1591	64.87	64.87	0.00	0.5166	0.7138	0.7138	0.00	121.82	13.39	0.62
0.0423	1305	0.8742	1.1408	67.17	66.07	1.10	0.5257	0.7067	0.7106	-0.0039	124.65	13.62	0.63
0.0905	1280	0.8769	1.1224	69.60	67.47	2.13	0.5351	0.7009	0.7068	-0.0059	127.98	13.89	0.65
0.1457	1255	0.8796	1.1039	72.18	69.13	3.06	0.5450	0.6951	0.7023	-0.0072	131.96	14.23	0.67
0.2097	1230	0.8823	1.0852	74.92	71.10	3.81	0.5552	0.6886	0.6970	-0.0084	136.77	14.65	0.69
0.2846	1205	0.8850	1.0664	77.82	73.52	4.30	0.5658	0.6813	0.6905	-0.0092	142.70	15.18	0.71
0.3738	1180	0.8877	1.0475	80.90	76.52	4.38	0.5770	0.6741	0.6824	-0.0083	150.13	15.86	0.73
0.4814	1155	0.8904	1.0284	84.19	80.37	3.82	0.5886	0.6649	0.6720	-0.0071	159.73	16.75	0.75
0.6141	1130	0.8931	1.0092	87.69	85.47	2.22	0.6007	0.6525	0.6582	-0.0057	172.53	17.97	0.76
0.7817	1105	0.8958	0.9899	91.42	92.55	-1.13	0.6133	0.6359	0.6391	-0.0032	190.40	19.68	0.78
1.0000	1040	0.8971	0.9330	103.06	103.06	0.00	0.6512	0.6108	0.6108	0.0000	217.37	22.02	0.84

Table 4: Chloropyriphos + P-xylene at 25°C ± 0.05°C.

Conc.(c)	V	ρ	Z	β_s	β_so	β_s- $\beta_{s/C}$	L_f	η	η_{sp}	η- $\eta_{sp/C}$	M_V	R	τ_s
0.0000	1312	0.8498	1.1149	68.36	68.36	0.00	0.5217	0.6145	0.6145	0.0000	124.94	13.67	0.56
0.0423	1284	0.8583	1.1021	70.67	69.22	1.45	0.5304	0.6075	0.6151	-0.0076	126.96	13.80	0.57
0.0905	1256	0.8668	1.0887	73.13	70.21	2.92	0.5396	0.6062	0.6159	-0.0097	129.47	13.97	0.59
0.1457	1228	0.8753	1.0749	75.76	71.39	4.37	0.5492	0.6061	0.6168	-0.0106	132.61	14.20	0.61
0.2097	1200	0.8838	1.0606	78.57	72.80	5.78	0.5593	0.6070	0.6178	-0.0108	136.54	14.51	0.64
0.2846	1172	0.8923	1.0458	81.59	74.51	7.08	0.5699	0.6081	0.6191	-0.0110	141.53	14.92	0.66
0.3738	1144	0.9008	1.0305	84.82	76.65	8.17	0.5811	0.6103	0.6207	-0.0104	147.95	15.47	0.69
0.4814	1116	0.9093	1.0148	88.30	79.39	8.92	0.5929	0.6135	0.6227	-0.0094	156.41	16.22	0.72
0.6141	1088	0.9178	0.9986	92.04	83.01	9.03	0.6053	0.6178	0.6254	-0.0076	167.88	17.26	0.76
0.7817	1060	0.9263	0.9819	96.08	88.05	8.03	0.6185	0.6281	0.6292	-0.0051	184.13	18.77	0.80
1.0000	1062	0.9282	0.9857	95.52	95.52	0.00	0.6167	0.6348	0.6348	0.0000	210.08	21.43	0.81

Table 5: Chloropyriphos + P-xylene at 30°C ± 0.05°C.

Conc.(c)	V	ρ	Z	β_s	β_so	β_s- $\beta_{s/C}$	L_f	η	η_{sp}	η- $\eta_{sp/C}$	M_V	R	τ_s
0.0000	1296	0.8304	1.0762	71.70	71.70	0.00	0.5389	0.5828	0.5828	0.0000	127.58	13.94	0.56
0.0423	1271	0.8384	1.0656	73.83	72.58	1.26	0.5469	0.5785	0.5841	-0.0056	130.01	14.08	0.57
0.0905	1246	0.8464	1.0546	76.10	73.60	2.50	0.5552	0.5772	0.5856	-0.0084	132.67	14.27	0.59
0.1457	1221	0.8544	1.0432	78.51	74.81	3.70	0.5639	0.5778	0.5873	-0.0095	135.98	14.53	0.60
0.2097	1196	0.8624	1.0314	81.06	76.25	4.81	0.5730	0.5793	0.5895	-0.0102	140.12	14.87	0.63
0.2846	1171	0.8704	1.0192	83.79	78.01	5.77	0.5826	0.5818	0.5920	-0.0103	145.35	15.32	0.65
0.3738	1146	0.8784	1.0066	86.68	80.21	6.48	0.5926	0.5858	0.5952	-0.0094	152.07	15.91	0.68
0.4814	1121	0.8864	0.9937	89.78	83.02	6.76	0.6030	0.5914	0.5994	-0.0080	160.91	16.71	0.71
0.6141	1096	0.8944	0.9803	93.08	86.74	6.34	0.6140	0.5983	0.6048	-0.0065	172.88	17.82	0.74
0.7817	1071	0.9024	0.9665	96.61	91.91	4.70	0.6256	0.6084	0.6124	-0.0040	189.81	19.42	0.78
1.0000	1050	0.9108	0.9563	99.59	99.59	0.00	0.6351	0.6236	0.6236	0.0000	215.20	21.87	0.83

Table 6: Chloropyriphos + P-xylene at 35°C ± 0.05°C.

Conc.(c)	V	ρ	Z	β_s	β_so	β_s- $\beta_{s/C}$	L_f	η	η_{sp}	η- $\eta_{sp/C}$	M_V	R	τ_s
0.0000	1282	0.8184	1.0492	74.35	74.35	0.00	0.5531	0.5584	0.5584	0.0000	129.73	14.09	0.55
0.0423	1258	0.8261	1.0392	76.49	75.25	1.24	0.5610	0.5562	0.5601	-0.0039	131.95	14.24	0.57
0.0905	1234	0.8338	1.0289	78.76	76.30	2.46	0.5693	0.5561	0.5620	-0.0059	134.68	14.44	0.58
0.1457	1210	0.8415	1.0182	81.17	77.55	3.62	0.5779	0.5570	0.5642	-0.0072	138.07	14.71	0.60
0.2097	1186	0.8492	1.0072	83.72	79.03	4.68	0.5963	0.5586	0.5670	-0.0084	142.30	15.06	0.62
0.2846	1162	0.8569	0.9957	86.43	80.85	5.58	0.6062	0.5611	0.5703	-0.0092	147.64	15.52	0.65
0.3738	1138	0.8646	0.9839	89.31	83.11	6.20	0.6165	0.5661	0.5744	-0.0083	154.50	16.13	0.67
0.4814	1114	0.8723	0.9717	92.38	86.00	6.38	0.6273	0.5726	0.5797	-0.0071	163.51	16.95	0.71
0.6141	1090	0.8800	0.9592	95.65	89.83	5.81	0.6273	0.5809	0.5867	-0.0057	175.71	18.08	0.74
0.7817	1066	0.8877	0.9463	99.13	95.16	3.97	0.6387	0.5932	0.5964	-0.0032	192.95	19.71	0.78
1.0000	1040	0.8971	0.9330	103.06	103.0	0.00	0.6512	0.6108	0.6108	0.0000	218.48	22.13	0.84

Result and Discussion

Present work covers an extensive study of solute–solvent interaction of chloropyriphos with aqueous organic sovlents as o-xylene and p-xylene. We have reported ultrasound velocity(v), density(ρ), and viscosity(η), of binary liquid mixture with help of experimental data, the following thermodynamic and acouetic properties

like isentropic compressibility (β_s), intermolecular free length(L_f) , molar volume (M_V), available volume (Va), shear's relaxation time(τ_s) have been calculated. All the system studied at various temperatures (25^{o}C, 30^{o}C and 35^{o}C).

The positive excess compressibility and negative viscosity concluded the non specific interaction between the molecules of Chloropyriphos in binary solvents. The excess intermolecular free length also being positive observed which also support the non specific interaction between the unlike molecules. The excess molar volume and available volume reported in the tables (1-6) as well as on figures (1-4). The continuos observation of above binary parameters also given the comparative conclusion of results. The positive excess compressibility increases from o-xylene to p-xylene.

The reported structure of Chloropyriphos pesticides, although has phosphorothioate group with two oxy-ethyl, three chlorine atoms and full filled nitrogen atom so pesticides must be in position to interact with unlike molecule Ortho methyl group xylene and Para methyl group of xylene. It will be possible that slight interaction may be possible due to phosphorothioate group of pesticides and bipolar nature of non-polar solvents like o-xylene and p-xylene. It is possible that associating nature of phosphorothioate group of pesticide activate the non polar group and molecules of unlike molecules so that least interaction with induced group or molecules. The above facts also observed in p-xylene because the positive excess compressibility is highest in p-xylene and least in o-xylene. Because p-xylene is less polar than o-xylene.

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