



SOLID STATE STUDIES ON PHENYL BUTAZONE DRUG

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Abstract

The electrical conductivity of the Phenylbutazone drug has been studied using impedance spectroscopic technique (IS). Conductivity as a function of temperature has been measured and reported. The transition has been interpreted in terms of molecular symmetry.

Introduction

Singularity- A breaking point in the evolution of the state of a system is known as singularity. The Big-Bang¹ from which our universe originated and the transition state in a chemical reaction are well known Phase transition² is another example of singularity.

Phenylbutazone is a synthetic, pyrazolone derivative. It is a nonhormonal anti-inflammatory, antipyretic compound useful in the management of inflammatory conditions.⁴⁻⁵

Experimental

- 1) FTIR spectrum of Phenylbutazone was recorded on Shimadzu 84,005 FTIR spectrophotometer using KBr matrix.⁶⁻¹⁰
- 2) Phenyl Butazone drug were taken and after grounding it in a mortar pestle the phenyl butazone was pelleted to form a pellet of diameter 1.294 cm. & thickness 0.474 cm. silver electrodes were polished on the surface for other transport characterization.
- 3) Electrical conductivity on a function of temperature was measured by Impedance spectroscopy technique (IS) using HIOKI LCR Bridge (model 353250) in the frequency range of 42 Hz to 5 MHz.

temp.(C)	temp (K)	Z'	cond.	1000/T	log(S)
24	297	23	0.015683939	3.367003367	-1.80454486
30	303	24	0.015030441	3.300330033	-1.823028265
40	313	21	0.017177647	3.194888179	-1.765036318
50	323	22	0.016396845	3.095975232	-1.785239704
60	333	23	0.015683939	3.003003003	-1.80454486
70	343	25	0.014429224	2.915451895	-1.840757032

80	353	25	0.014429224	2.83286119	-1.840757032
90	363	27	0.013360392	2.754820937	-1.874180788
100	373	18	0.020040589	2.680965147	-1.698089529
110	383	19	0.018985821	2.610966057	-1.721570625

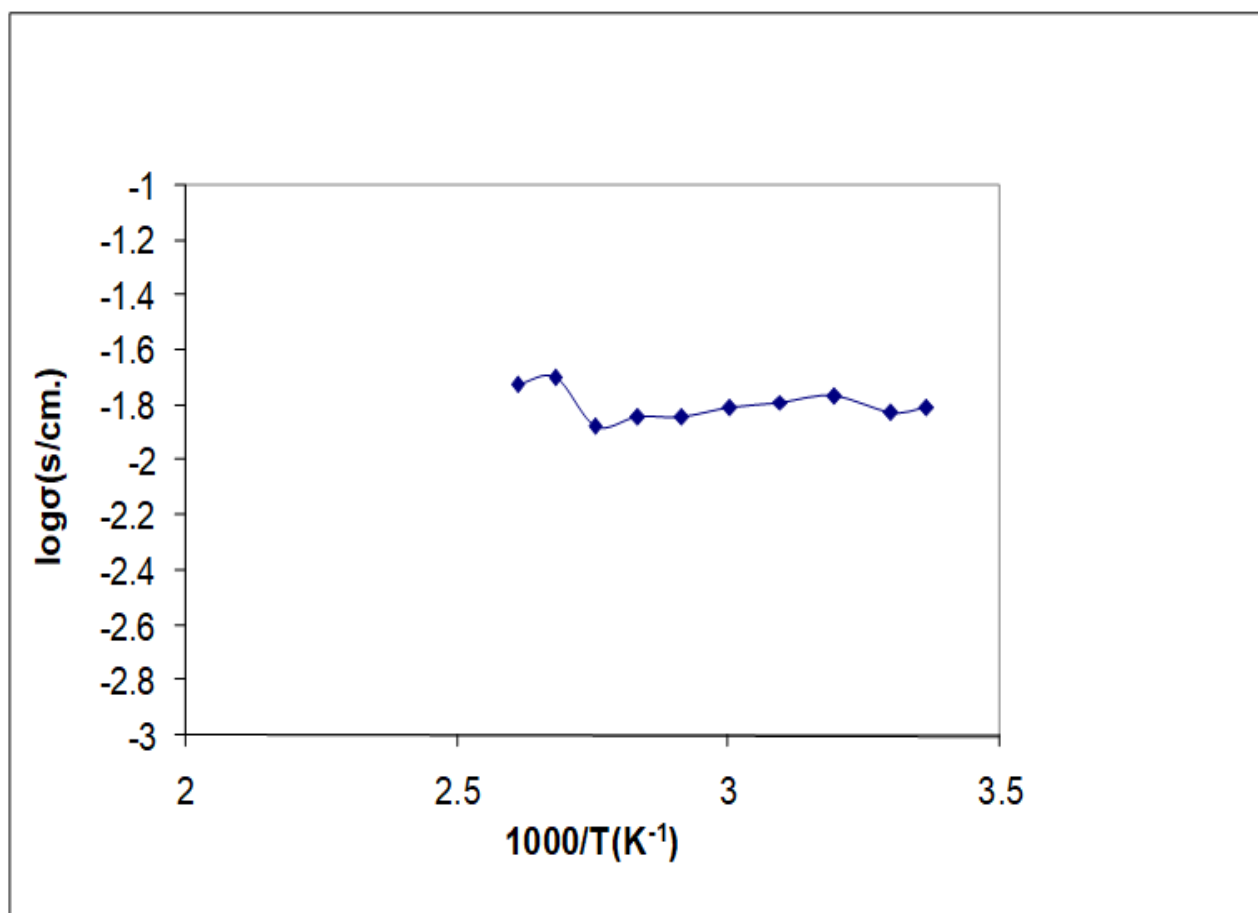
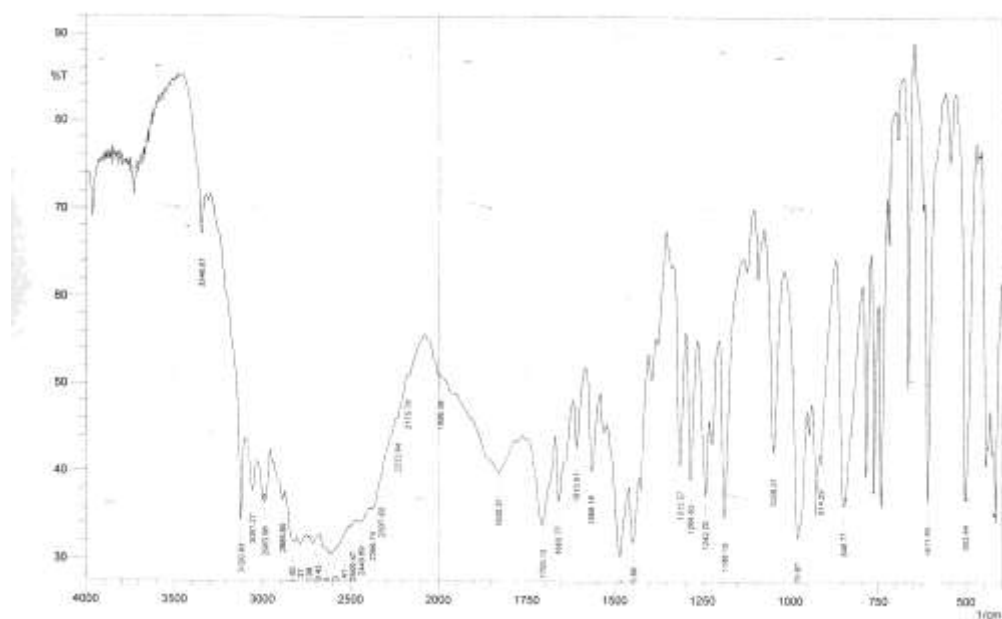


Fig.-1 Variation of conductivity on a function of temperature of phenylbutazone

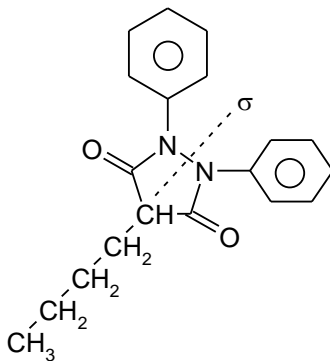


	Peak	Intensity
1	503.44	28.659
2	611.45	28.165
3	667.39	55.335
4	742.62	27.138
5	763.84	30.204
6	848.71	27.039
7	927.79	25.141
8	979.87	19.708
9	1049.31	40.036
10	1188.19	24.219
11	1242.2	29.487
12	1284.63	33.306
13	1313.57	36.724
14	1446.66	18.728
15	1485.24	15.839
16	1568.18	35.485
17	1660.77	28.159
18	1705.13	22.637
19	1830.51	34.879
20	1996.39	57.683
21	2175.78	57.825
22	2233.64	47.987
23	2337.8	32.327
24	2366.74	26.544
25	2443.89	23.034
26	2509.47	21.902
27	2565.41	17.863
28	2580.84	17.244
29	2600.13	16.469
30	2621.35	16.198
31	2700.43	18.684
32	2710.08	18.314
33	2740.94	19.523
34	2783.37	18.045
35	2821.95	18.418
36	2885.6	28.49
37	2983.98	27.73
38	3057.27	30.685
39	3120.93	23.659

Fig.-2 FTIR spectrum of Phenylbutazone

Results and Discussion

Phenylbutazone is a drug used for treating spondylitis³. Impedance measurements at different temperatures indicate a phase transition above room temperature. Attempt has been made to understand this transition in terms of molecular symmetry. A plane of symmetry can be identified in this molecule and a point group can be assigned C_s



It is possible for this molecule to pass into chair like structure which has point group C_2 . The molecule loses the plane but acquires an axis of symmetry. In objects point symmetry can be considered higher than axis symmetry and that in turn is higher than plane symmetry. In this way this molecule can acquire a conformation of higher symmetry in high-temperature phase. About forty infrared

absorption bands have been observed for this molecule at room temperature. Group theory predicts reduction in the number of bands if a conformation of higher symmetry is acquired. This can be confirmed by recording an infrared or Laser Raman spectrum above the transition temperature.

Conclusion

Variable-temperature impedance measurements indicate existence of a phase transition above room temperature. Symmetry elements have been identified and point groups assigned in the two phases. This phase transition is possibly the one in which the molecule slips from lower symmetry to higher symmetry ($C_s \rightarrow C_2$ point group). The proposal mechanism needs to be confirmed by further investigations.

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