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Vibrational Spectroscopic Studies, Experimental and Computational calculations of L-Glutamine Potassium Carbonate

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Abstract

The single crystals of L-Glutamine Potassium Carbonate have been grown by solution growth using slow evaporation technique. The vibrational wave numbers and corresponding vibrational assignments of L-Glutamine Potassium Carbonate are examined theoretically using the Gaussian09 set of quantum chemistry codes. Comparison of the observed IR and Raman spectra with the calculated results by HF and DFT method is found in agreement with the experimental data. Theoretical infrared and Raman intensities are reported. The FT-IR and FT-Raman spectrum of L-Glutamine Potassium Carbonate was recorded in the region 4000–100 cm^{-1}. Quantum chemical calculations of energies, geometrical structure and vibrational wave numbers of L-Glutamine Potassium Carbonate were carried out by HF and DFT methods with 3-21 G (d, p) basis sets and the corresponding results were tabulated. The difference between the observed and theoretical wave number values of most of the fundamentals is very small. A detailed interpretation of the infrared and Raman spectra of L-Glutamine Potassium Carbonate is also reported based on total energy distribution. The grown crystals were characterized by single crystal X-ray diffraction (XRD) to study the crystal structure. The presence of functional groups was identified through FT-IR and FT-Raman technique. The optical study exposed that the crystal has high transmission with lower cut off wavelength of 208.03 nm. Vickers micro-hardness test has done on the crystal and this shows that the crystal has greater physical strength.

Key words: Hartee-Fock; DFT; L-Glutamine Potassium Carbonate; NLO; XRD

1. Introduction

In crystal growth research, for the past four decades, activities have been focused towards the NLO (Non Linear Optical) crystals by researchers. In recent times, numbers of semi-organic crystals have been walk around, owing to their optoelectronic technologies, good mechanical strength, nonlinearity nature [1-4]. In recent research, semi-organic crystals with large nonlinear susceptibility, good optical transparency with high hardness have been identified. Semi-organic complex of L-Glutamine Potassium Carbonate with good optical nonlinearity combined with the physical austerity of inorganic compound have been useful for device applications. In the present work, we report a new semi-organic NLO material, L-Glutamine Potassium Carbonate which has proficient optical second harmonic generation. The title compound crystal thus has high resourceful optical quality for wide applications in the field of laser communication, laser technology and data storage tools [5].

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2. Experimental and Computational Methods

Solution is a homogeneous mixture of solute and solvent. Here the experimental crystal has been grown, using the preparation of two types of solutions in the following way. At first 14.615 gm of L-Glutamine Amino acid is dissolved in 100 ml of distilled water at room temperature by using magnetic stirrer and kept in a separate beaker. This is considered as a solution 1. In another beaker 13.812 gm of potassium carbonate is dissolved in 100 ml of distilled water at room temperature by using magnetic stirrer and kept in another beaker. This is considered as a solution 2. Then these two solutions are mixed with one another and stirred for more than one hour. Finally the solutions were mixed well which gives a single solution. Then the solution is taken in a beaker and the mouth of the beaker should be covered with polythene paper and 6 or 7 holes are made on it. Then the solution is left undisturbed.

The solution is kept under constant evaporation by keeping it in constant temperature bath. As a result of slow evaporation the excess of solute that got deposited at the bottom of the beaker results in the formation of seed crystals in a few days. After 100-110 days L-Glutamine Potassium Carbonate crystals are obtained (Figure 1).

The FT-IR spectrum was recorded using a Perkin-Elmer FT-IR spectrometer. The spectral resolution was 4 cm. Standard KBr technique with 1 mg sample per 300 mg KBr was used. The FT-Raman spectrum was obtained on a Bruker IFS 66V NIR-FT instrument equipped with a FRA 106 Raman module. A Nd/YAG laser at 1064 nm with an output on 300 mW was used as the exciting source. The absorption spectrum of title compound is recorded using Varion Cary 5E UV-Vis-NIR spectrophotometer in the range 200 – 700 nm with high resolution.

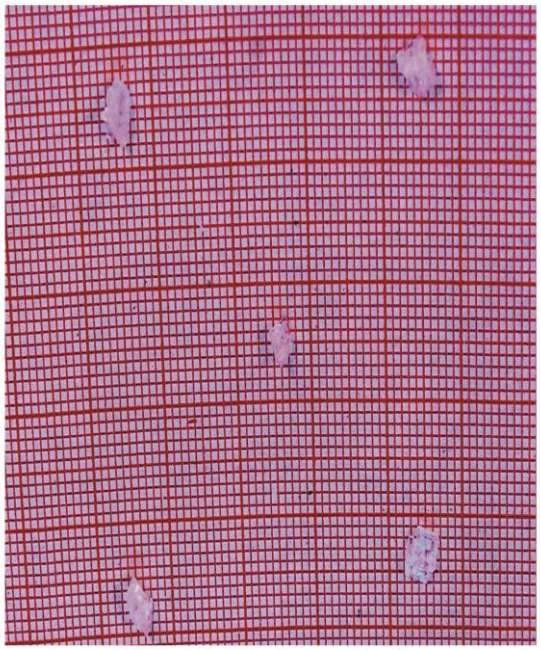

Figure 1: Photograph of
L-Glutamine Potassium Carbonate Crystals

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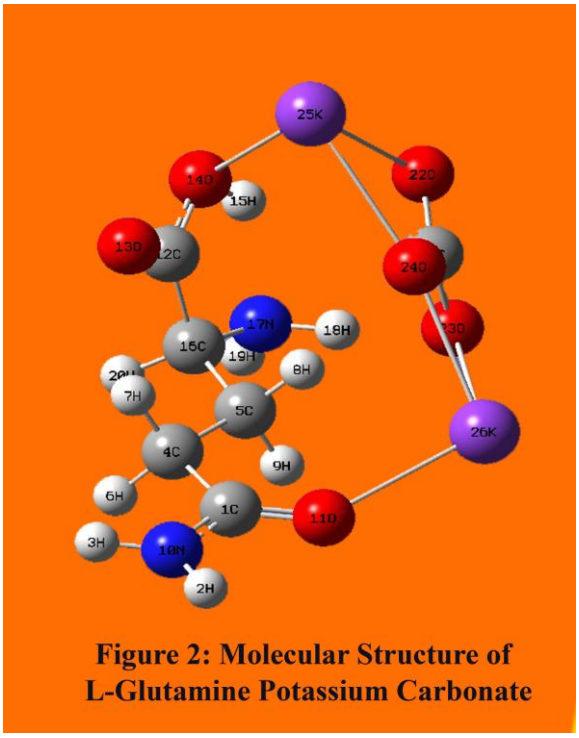

Figure 2: Molecular Structure of L-Glutamine Potassium Carbonate

Computational calculations of L-Glutamine Potassium Carbonate are carried out with GAUSSIAN O9 using the HF and DFT methods with 3-21 G (d, p) basis sets to predict the molecular structure and vibrational wave numbers. Molecular geometry was fully optimized by Berny's optimization algorithm using redundant internal coordinates. Harmonic vibrational wave numbers are calculated using the analytic second derivatives to confirm the convergence to minima on the potential surface. The wave number values computed at the HF and DFT level contain known systematic errors due to the negligence of electron correlation. Parameters corresponding to optimized geometry of L-Glutamine Potassium Carbonate (Figure 2) are given in Table (1). The absence of imaginary wave numbers on the calculated vibrational spectrum confirms that the structure corresponds to minimum energy.

The observed (FT-IR & FT-Raman) and calculated vibrational frequencies and vibrational assignments are submitted in Table (2) and (3). Experimental and simulated spectra of IR and Raman are presented in the Figures (3) and (4), respectively.

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Table (1): Optimized geometrical parameters for L-Glutamine Potassium Carbonate computed at HF, DFT (B3LYP& B3PW91), CAM - B3LYP and LSDA with 3-21G (d, p) basis sets

Geometrical Parameters	Methods				
	HF	B3LYP	CAM-B3LYP	B3PW91	LSDA
	3-21G	3-21G	3-21G	3-21G	3-21G
Bond length(Å)					
(C1 - C4)	1.5175	1.5204	1.5159	1.5194	1.4918
(C1 - N10)	1.3464	1.3596	1.3513	1.3559	1.3517
(C1 - O11)	1.2304	1.2547	1.2471	1.2522	1.2574
(H2 - N10)	0.9978	1.0144	1.0135	1.0142	1.0238
(H3 - N10)	0.9956	1.0126	1.0104	1.0112	1.0223
(C4 - C5)	1.5287	1.5325	1.5392	1.5419	1.539
(C4 - H6)	1.0869	1.0985	1.092	1.0945	1.1116
(C4 - H7)	1.0822	1.0999	1.0948	1.0987	1.1195
(C5 - H8)	1.0779	1.09	1.0866	1.0896	1.1058
(C5 - H9)	1.0822	1.0975	1.0959	1.0987	1.1075
(C5 - C16)	1.5431	1.5386	1.5281	1.5315	1.5398
(C12 - O13)	1.2162	1.282	1.287	1.2911	1.2721
(C12 - O14)	1.3333	1.28	1.2612	1.2678	1.2847

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(C12 - C16)	1.5338	1.5735	1.5537	1.5612	1.5588
(O14 - H15)	0.9954	1.8933	2.6332	2.6436	1.6554
(O14 - K25)	2.7093	2.6997	2.5955	2.6337	2.5819
(C16 - N17)	1.47	1.509	1.5005	1.5045	1.4939
(C16 - H20)	1.0846	1.0993	1.0947	1.0973	1.1071
(N17 - H18)	1.0324	1.5431	1.5995	1.5638	1.2659
(N17 - H19)	1.0022	1.0252	1.0211	1.0226	1.0325
(C21 - O22)	1.2682	1.2614	1.2784	1.2862	1.2673
(C21 - O23)	1.3055	1.4241	1.3977	1.4025	1.3734
(C21 - O24)	1.3286	1.3034	1.2753	1.2809	1.3207
(O22 - K25)	2.5401	2.6151	2.5635	2.5925	2.5312
(O24 - K26)	2.555	2.5682	2.6023	2.6458	2.5065
Bond angle (°)					
(C4 - C1 - N10)	115.0913	114.9511	116.2316	115.9114	113.9478
(C4 - C1 - O11)	123.213	123.6307	121.9972	122.3014	124.7449
(N10 - C1 - O11)	121.6956	121.4143	121.7567	121.7736	121.2527
(C1 - C4 - C5)	110.7264	111.5312	110.8109	110.8617	109.3059
(C1 - C4 - H6)	108.2599	109.4169	111.8245	112.0532	114.0625
(C1 - C4 - H7)	109.1507	110.5577	106.1442	106.192	110.5779

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(C5 - C4 - H6)	111.4196	111.704	111.8437	111.761	105.1056
(C5 - C4 - H7)	109.0908	104.6069	105.9801	105.6875	110.1907
(H6 - C4 - H7)	108.1307	108.9191	109.9117	109.9365	107.4376
(C4 - C5 - H8)	109.4642	108.2991	109.0738	109.0418	108.2403
(C4 - C5 - H9)	109.7732	110.3279	110.26	110.2073	107.9997
(C4 - C5 - C16)	114.4511	112.9229	114.1745	114.1315	115.033
(H8 - C5 - H9)	108.9746	109.3908	107.2058	107.0681	108.6
(H8 - C5 - C16)	106.5159	106.2434	106.1085	106.3053	107.3446
(H9 - C5 - C16)	107.4987	109.5253	109.7122	109.7805	109.4651
(C1 - N10 - H2)	119.2117	119.2335	118.8852	119.0101	119.3954
(C1 - N10 - H3)	122.1242	121.617	122.0153	121.979	120.5689
(H2 - N10 - H3)	118.6439	119.0689	119.0899	119.0009	119.9929
(O13 - C12 - O14)	120.8367	126.1283	125.3964	125.6481	125.9009
(O13 - C12 - C16)	125.1296	118.0472	118.3488	118.5175	120.5538
(O14 - C12 - C16)	113.913	115.5493	116.1671	115.7657	113.4626
(C12 - O14 - H15)	107.925	88.8144	66.574	66.314	91.6072
(C12 - O14 - K25)	93.4044	83.0078	90.4503	90.4543	84.2696
(H15 - O14 - K25)	112.801	110.6493	88.9941	87.3645	109.9016
(C5 - C16 - C12)	108.2415	109.499	112.7424	113.2755	115.5639

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(C5 - C16 - N17)	112.2997	110.7079	107.7433	107.6876	112.5922
(C5 - C16 - H20)	110.9925	110.7138	111.9339	111.8053	108.9
(C12 - C16 - N17)	106.8225	105.4533	106.7912	106.7137	103.9015
(C12 - C16 - H20)	107.7852	109.3523	106.5747	106.4226	106.0636
(N17 - C16 - H20)	110.4816	110.969	110.9691	110.8493	109.4786
(C16 - N17 - H18)	112.6266	109.8511	107.2576	108.4857	108.554
(C16 - N17 - H19)	114.2743	112.2801	112.9675	112.7966	113.5974
(H18 - N17 - H19)	113.632	114.5751	123.6033	122.9903	115.0125
(O22 - C21 - O23)	123.011	118.9256	117.4701	117.5037	119.8354
(O22 - C21 - O24)	119.6206	126.3008	125.9955	125.9541	123.8714
(O23 - C21 - O24)	117.1438	114.5725	116.2789	116.3469	116.0613
(C21 - O22 - K25)	94.2293	89.8643	89.131	89.478	89.0464
(C21 - O24 - K26)	94.4709	99.0199	91.8616	91.6305	94.3526
(O14 - K25 - O22)	67.7363	76.1352	75.0994	75.6342	67.6634
Dihedral angle (°)					
(N10 - C1 - C4 - C5)	-178.4863	-175.3239	-132.048	-130.5871	-83.9347
(N10 - C1 - C4 - H6)	-56.0732	-51.2267	-6.5279	-4.9641	33.377
(N10 - C1 - C4 - H7)	61.4084	68.7312	113.3299	115.0839	154.5884
(O11 - C1 - C4 - C5)	1.5936	5.3881	49.3168	50.7308	93.3968

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(O11 - C1 - C4 - H6)	124.0067	129.4853	174.8368	176.3538	-149.2915
(O11 - C1 - C4 - H7)	-118.5117	-110.5568	-65.3053	-63.5982	-28.0801
(C4 - C1 - N10 - H2)	-179.4324	-178.1435	-178.528	-178.6061	177.143
(C4 - C1 - N10 - H3)	-1.0878	-1.4391	2.6123	2.5575	-5.2375
(O11 - C1 - N10 - H2)	0.489	1.1618	0.1108	0.0836	-0.2922
(O11 - C1 - N10 - H3)	178.8337	177.8662	-178.7489	-178.7529	177.3273
(C1 - C4 - C5 - H8)	-57.0622	-58.2107	-35.2241	-35.4583	-68.8419
(C1 - C4 - C5 - H9)	62.5097	61.4875	82.2443	81.7935	48.5578
(C1 - C4 - C5 - C16)	-176.5288	-175.5803	-153.7141	-154.1481	171.1355
(H6 - C4 - C5 - H8)	-177.6133	178.9908	-160.7333	-161.2448	168.335
(H6 - C4 - C5 - H9)	-58.0414	-61.311	-43.2649	-43.993	-74.2653
(H6 - C4 - C5 - C16)	62.9201	61.6213	80.7767	80.0653	48.3125
(H7 - C4 - C5 - H8)	63.0789	61.3221	79.5009	79.187	52.8689
(H7 - C4 - C5 - H9)	-177.3492	-178.9797	-163.0307	-163.5611	170.2686
(H7 - C4 - C5 - C16)	-56.3877	-56.0474	-38.9891	-39.5028	-67.1537
(C4 - C5 - C16 - C12)	74.4552	73.3778	53.9908	52.4404	-10.9727
(C4 - C5 - C16 - N17)	-167.8654	-170.7703	171.5723	170.2012	108.2037
(C4 - C5 - C16 - H20)	-43.6402	-47.2682	-66.1579	-67.797	-130.181
(H8 - C5 - C16 - C12)	-46.6509	-45.1953	-66.1729	-67.7932	-131.4878

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(H8 - C5 - C16 - N17)	71.0285	70.6566	51.4086	49.9676	-12.3114
(H8 - C5 - C16 - H20)	-164.7463	-165.8413	173.6783	171.9694	109.304
(H9 - C5 - C16 - C12)	-163.3356	-163.2446	178.3256	176.7275	110.8154
(H9 - C5 - C16 - N17)	-45.6562	-47.3927	-64.0929	-65.5117	-130.0083
(H9 - C5 - C16 - H20)	78.569	76.1094	58.1769	56.4901	-8.3929
(O13 - C12 - O14 - H15)	167.412	158.7835	124.257	124.25	163.0042
(O13 - C12 - O14 - K25)	52.1178	47.812	35.5484	37.3278	53.1618
(C16 - C12 - O14 - H15)	-8.7929	-15.0381	-52.2681	-52.6736	-13.6811
(C16 - C12 - O14 - K25)	-124.087	-126.0096	-140.9767	-139.5958	-123.5235
(O13 - C12 - C16 - C5)	-46.0033	-31.3645	16.9552	17.4624	-35.1386
(O13 - C12 - C16 - N17)	-167.1372	-150.5132	-101.1862	-100.8644	-158.9941
(O13 - C12 - C16 - H20)	74.1197	90.1058	140.1403	140.7163	85.6182
(O14 - C12 - C16 - C5)	130.012	142.983	-166.2631	-165.3826	141.7436
(O14 - C12 - C16 - N17)	8.8781	23.8343	75.5955	76.2906	17.8882
(O14 - C12 - C16 - H20)	-109.865	-95.5467	-43.078	-42.1287	-97.4995
(C12 - O14 - K25 - O22)	108.8534	102.818	68.1831	68.1069	107.8507
(H15 - O14 - K25 - O22)	-2.2136	16.7457	1.6223	1.8431	18.2146
(C5 - C16 - N17 - H18)	-24.6922	-25.4647	-49.9218	-50.07	-26.8498
(C5 - C16 - N17 - H19)	106.9423	103.273	89.6379	89.6841	102.4454

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(C12 - C16 - N17 - H18)	93.8268	92.8773	71.4457	71.8552	98.9159
(C12 - C16 - N17 - H19)	-134.5387	-138.385	-148.9945	-148.3906	-131.789
(H20 - C16 - N17 - H18)	-149.2002	-148.8196	-172.7851	-172.6623	-148.1359
(H20 - C16 - N17 - H19)	-17.5657	-20.0819	-33.2254	-32.9082	-18.8408
(O23 - C21 - O22 - K25)	154.7091	138.6908	137.1378	137.2225	138.5243
(O24 - C21 - O22 - K25)	-19.6873	-35.8582	-36.8159	-37.4927	-35.7197
(O22 - C21 - O24 - K26)	-170.4599	-176.4953	140.433	140.6891	-170.3365
(O23 - C21 - O24 - K26)	14.8197	8.7502	-33.5843	-34.0802	15.2211
(C21 - O22 - K25 - O14)	-94.6085	-99.2516	-109.2535	-108.5887	-109.2977

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Table (2): Observed and calculated FT-IR frequencies of L-Glutamine computed at HF, DFT (B3LYP& B3PW91) and CAM - B3LYP with 3-21G (d,p) basis sets

Observed frequency (cm^{-1})		Methods					Vibrational assignments
		HF	B3LYP	CAM-B3LYP	B3PW91	LSDA	
FTIR	FT Raman	3-21G	3-21G	3-21G	3-21G	3-21G	
-	-	3898	3652	3688	3684	3576	N-H asym. stretching
-	-	3772	3524	3561	3551	3439	N-H sym. stretching
-	-	3758	3451	3513	3497	3400	N-H sym. stretching
3199m	3000w	3432	3217	3266	3195	3038	N-H sym. stretching
-	2990w	3320	3161	3225	3193	2999	N-H asym. stretching
-	2920m	3282	3073	3155	3129	2972	N-H asym. stretching
-	2870w	3238	3046	3098	3071	2944	N-H asym. stretching
2528w	-	3232	3029	3095	3065	2821	N-H stretching
2398w	-	3220	3022	3085	3057	2746	N-H stretching
2239w	-	3201	2150	2469	2297	1794	C=N stretching
1879w	-	1909	1710	1768	1758	1706	C=C stretching
-	-	1901	1703	1748	1724	1700	N-H bending
1715w	1620vs	1851	1670	1708	1699	1650	C=O stretching
1624w	1570w	1812	1667	1684	1671	1598	C=O stretching

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-	-	1710	1595	1671	1644	1580	N-H bending
1500w	1500w	1645	1571	1566	1547	1567	N-H bending
-	-	1633	1557	1538	1519	1517	C-H bending
-	1460w	1596	1532	1525	1516	1479	C-H bending
1422w	1450w	1527	1435	1441	1422	1441	C-H bending
-	1410w	1517	1399	1426	1400	1405	C-H bending
-	1380m	1488	1389	1410	1383	1369	C-H bending
-	-	1475	1349	1386	1361	1349	C-H bending
1310w	1300m	1437	1342	1366	1337	1319	C-N stretching
-	-	1422	1314	1347	1328	1310	O=C=O stretching
-	-	1412	1292	1336	1308	1295	C-H bending
-	1260m	1362	1277	1322	1300	1259	C-N stretching
-	1220m	1333	1262	1272	1257	1226	C-N stretching
-	-	1307	1203	1227	1217	1200	C-H bending
-	-	1240	1178	1196	1207	1141	N-H bending
1125m	1150w	1215	1147	1150	1134	1120	C-O stretching
-	-	1177	1124	1112	1097	1080	N-H bending
-	-	1126	1079	1069	1052	1074	C=N stretching
-	-	1110	1060	1055	1041	1026	N-H bending
1019m	-	1074	1000	1031	1016	1010	C-O stretching

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-	1040w	1058	990	967	954	967	C-O stretching
-	940vw	971	913	956	945	952	CH_2 wagging
901m	-	935	865	899	883	925	CH_2 wagging
859m	860vs	928	852	864	848	839	C-H bending
-	-	902	823	811	800	811	C-H bending
-	-	866	794	807	792	799	C=O bending
-	-	816	768	784	774	773	C=O stretching
-	-	748	691	767	759	754	N-H stretching
-	-	743	659	679	666	702	O=C=O bending
-	-	726	644	664	657	669	O-K stretching
-	-	690	625	648	640	637	N-H bending
616m	-	630	586	629	617	616	C=O bending
569w	550w	623	559	581	571	582	C-C=O bending
-	-	599	554	573	563	576	N-H bending
-	-	571	539	555	547	573	N-H bending
-	-	543	526	517	509	543	N-H bending
499w	490vs	520	516	469	460	528	C=O stretching
-	480vs	407	401	389	386	486	C=O stretching
-	470vs	399	388	339	334	436	C=O stretching
-	350vs	336	330	318	319	417	O=C=O bending

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-	330m	276	296	288	278	316	O=C=O bending
-	260vs	272	261	277	267	258	O-K stretching
-	-	269	231	250	229	255	O-K stretching
-	200vs	253	222	240	214	246	O-K stretching
-	-	225	207	223	207	218	CH_2 bending
-	-	188	199	219	201	215	O-K stretching
-	180m	178	179	202	186	197	O-K stretching
-	-	174	170	191	179	190	O-K stretching
-	150m	157	164	181	168	177	O-K stretching
-	-	144	141	167	149	165	O=C=O bending
-	-	125	118	142	132	139	O=C=O bending
-	110w	115	107	136	128	128	O-K stretching
-	-	104	103	130	120	112	K-O-K bending
-	-	88	98	117	108	104	O-K-O bending
-	-	84	91	104	101	94	O-K-O bending
-	-	67	75	93	87	70	NH_2 bending
-	-	57	65	78	74	51	O=C=O bending
-	-	38	36	44	43	41	NH_2 bending

s – Strong; m–Medium; w – Weak; vs – Very Strong; vw – Very Weak;

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Table (3): Calculated Vibrational frequencies of L-Glutamine Potassium Carbonate computed at HF, DFT (B3LYP& B3PW91), CAM - B3LYP and LSDA with 3-21G (d, p) basis sets

S. No.	Methods				
	Calculated Vibrational frequencies				
	HF 3-21 G	B3LYP 3-21 G	CAM-B3LYP 3-21 G	B3PW91 3-21 G	LSDA 3-21 G
1	3898	3652	3688	3684	3576
2	3772	3524	3561	3551	3439
3	3758	3451	3513	3497	3400
4	3432	3217	3266	3195	3038
5	3320	3161	3225	3193	2999
6	3282	3073	3155	3129	2972
7	3238	3046	3098	3071	2944
8	3232	3029	3095	3065	2821
9	3220	3022	3085	3057	2746
10	3201	2150	2469	2297	1794
11	1909	1710	1768	1758	1706
12	1901	1703	1748	1724	1700
13	1851	1670	1708	1699	1650
14	1812	1667	1684	1671	1598
15	1710	1595	1671	1644	1580
16	1645	1571	1566	1547	1567
17	1633	1557	1538	1519	1517
18	1596	1532	1525	1516	1479
19	1527	1435	1441	1422	1441
20	1517	1399	1426	1400	1405
21	1488	1389	1410	1383	1369
22	1475	1349	1386	1361	1349
23	1437	1342	1366	1337	1319
24	1422	1314	1347	1328	1310
25	1412	1292	1336	1308	1295
26	1362	1277	1322	1300	1259
27	1333	1262	1272	1257	1226
28	1307	1203	1227	1217	1200
29	1240	1178	1196	1207	1141

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30	1215	1147	1150	1134	1120
31	1177	1124	1112	1097	1080
32	1126	1079	1069	1052	1074
33	1110	1060	1055	1041	1026
34	1074	1000	1031	1016	1010
35	1058	990	967	954	967
36	971	913	956	945	952
37	935	865	899	883	925
38	928	852	864	848	839
39	902	823	811	800	811
40	866	794	807	792	799
41	816	768	784	774	773
42	748	691	767	759	754
43	743	659	679	666	702
44	726	644	664	657	669
45	690	625	648	640	637
46	630	586	629	617	616
47	623	559	581	571	582
48	599	554	573	563	576
49	571	539	555	547	573
50	543	526	517	509	543
51	520	516	469	460	528
52	407	401	389	386	486
53	399	388	339	334	436
54	336	330	318	319	417
55	276	296	288	278	316
56	272	261	277	267	258
57	269	231	250	229	255
58	253	222	240	214	246
59	225	207	223	207	218
60	188	199	219	201	215
61	178	179	202	186	197
62	174	170	191	179	190
63	157	164	181	168	177
64	144	141	167	149	165
65	125	118	142	132	139
66	115	107	136	128	128

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67	104	103	130	120	112
68	88	98	117	108	104
69	84	91	104	101	94
70	67	75	93	87	70
71	57	65	78	74	51
72	38	36	44	43	41

3. Results and Discussion

3.1 Molecular Geometry Analysis

The optimized molecular structure of the molecule is obtained from Gaussian 09 and Gauss view program and is shown in Figure (2). The molecule contains two potassium, two nitrogen, six carbon, six oxygen and ten hydrogen atoms linked with coordination covalent bond. The comparative optimized structural parameters such as bond lengths, bond angles and dihedral angles are listed in Table (1). Concerning the bond distances the carbon-carbon and carbon-hydrogen bond lengths are close to the experimental values reported for amino acids in the gaseous state [6-7] namely 1.081Å (C-H), 1.526 Å (C-C) and 1.071 Å (C-H), 1.522 Å (C-C). With regard to the carbon-carbon distances, the HF results are sensitive to the influence of the oxygen atom, thus decreasing the C1– C4 length with respect to the central C-C bonds. Concerning the bond angles, the optimized values of NH_2 and COOH moieties compare well with previous results reported for other amino acids. As an example, the bond angles of the NH_2 and COOH moieties are nearer to the data reported for the title molecule from computational calculations [8] namely 126.1° (O-C-O), 111.8° (O-C-C), 122.1° (O=C-C) and 111.5° (C-O-H) for the carboxylic group and 113.6° (C-C-N), 112.9° (mean for the two C-N-H) and 110.5° (H-N-H) for the amino group. The computational calculation data values (Table 1), for the carboxylic acid, C12–O14 = 1.3333 Å, C12–O13 =1.2162 Å, O14–H15 = 0.9954 Å are closer to the theoretical results obtained for the title molecule [9], namely 1.361 Å (C-O) and 0.965 (O-H) and for L-Glutamine potassium carbonate namely 1.3055 Å (C21-O23) and 0.9954 Å (O14-H15). However, the DFT level of theory, in general slightly over estimates bond lengths but it yields bond angles which are in excellent agreement with the HF method.

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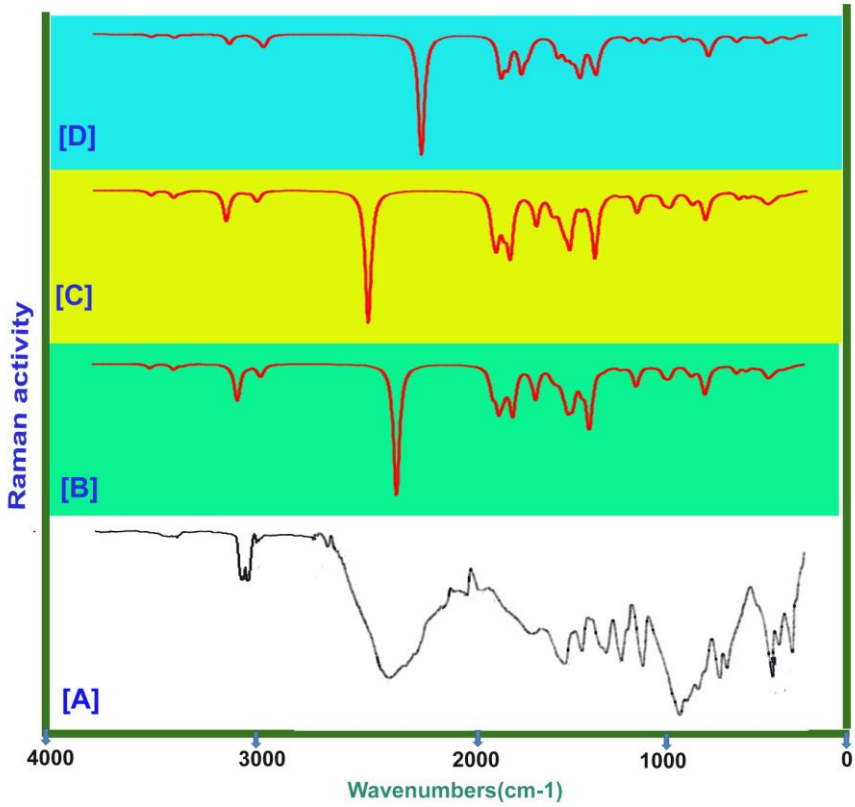

Figure 3:Experimental[A] and calculated[B,C&D] FT-IR spectra of L-Glutamine Potassium Carbonate

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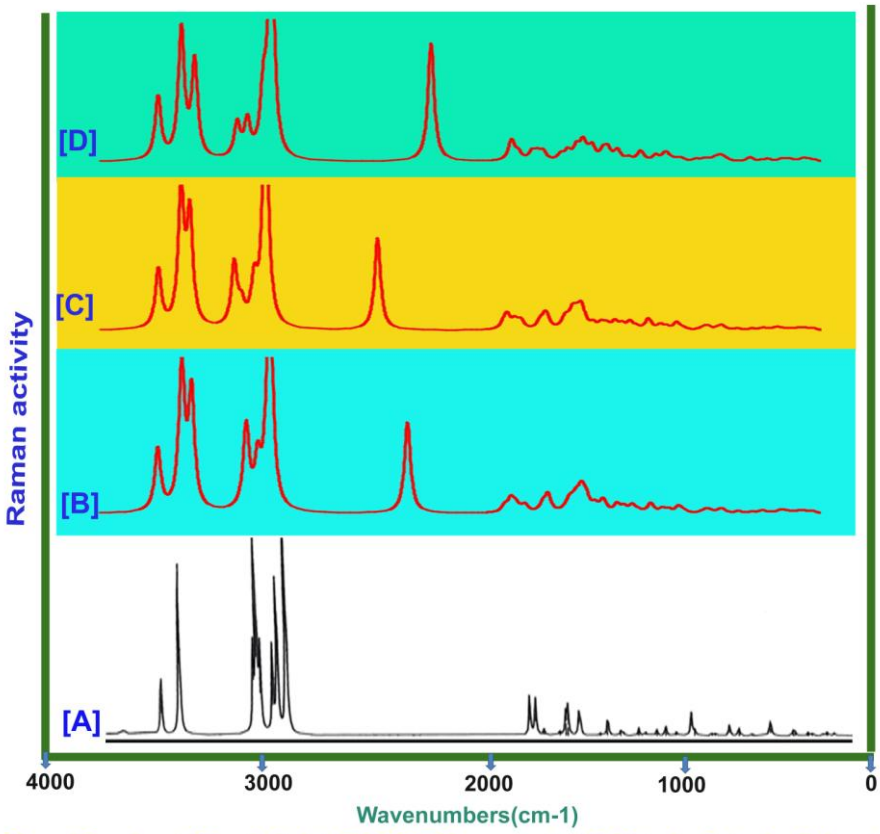

Figure 4:Experimental[A] and calculated[B,C&D] FT-Raman spectra of L-Glutamine Potassium Carbonate

3.2 Vibrational Analysis

The L-Glutamine potassium carbonate molecule consists of 26 atoms, which undergoes 72 normal modes of vibrations. The harmonic vibrational frequencies (theoretical and experimental) calculated at HF and DFT levels using the 3-21 G (d, p) basis sets and the observed FT-IR and FT-Raman frequencies for various modes of vibrations have been presented. The experimental and calculated frequencies and their assignments are presented in the Tables (2) and (3) and their experimental and simulated spectra of IR and Raman are presented in the Figures (3) and (4) respectively.

3.2.1 N–H Vibrations

In primary amines, usually the N–H stretching vibrations occur. The NH_2 group has two vibrations one is being asymmetric and other symmetric. The frequency of asymmetric vibration is higher than that of symmetric one. In the present study, the asymmetric and symmetric of N–H stretching is assigned at 3199, 3000, 2990, 2920, 2870, 2528 and 2398 cm^{-1} in FTIR and FT Raman respectively. The N–H bending vibrations of the present compound are observed at 1500 cm^{-1}.

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3.2.2 C=N and C–N VIBRATIONS

The C=N stretching vibrations usually occur in the region around 2250 cm^{-1}. The C=N stretching vibrations of the present compound are observed with weak intensity at 2259 cm^{-1}. The C–N stretching mode, the title compound is assigned to the wave number observed in weak and medium intensity at 1310, 1300, 1260 and 1220 cm^{-1} in the infrared and Raman spectra, respectively. This assignment is in line with the literature and most of the bands are observed in both IR and Raman spectra.

3.2.3 C=O and C–O Vibrations

The Carbonyl group vibrational frequencies are considered to be significant in the vibrational spectra of ketones, and for this reason, such bands have been the subject of extensive studies. The intensity of these bands can increase because of conjugation, therefore, leads to the intensification of the Raman lines as well as the increased infrared band intensities. The carbonyl asymmetric and other symmetric stretching vibrations in ketones are in the expected region. In this work, a strong, medium and weak bands at 1715, 1624, 1620, 1570, 616, 499, 490, 480, and 470 cm^{-1} in IR and Raman has been assigned to C=O stretching vibration. The carbonyl vibrations proposed in this study, though lie within the literature values. The C–O stretching mode, the title compound is assigned to the wave number which is observed in weak and medium intensity at 1150, 1125, 1040 and 1019 cm^{-1} in the infrared and Raman spectra, respectively.

3.2.4 C–H Vibrations

The C-H in-plane and out-of-plane bending vibrations generally lies in the range 1000 - 1300 cm^{-1} and 1000 - 675 cm^{-1} [10-13] respectively. In the present case, C-H in-plane bending vibrations are identified at 1460, 1450, 1422, 1410 & 1380 cm^{-1} and C-H out-of-plane bending vibrations are observed at 860 & 859 cm^{-1}. All these bands are located in the crest of the expected range which may also be due to all the three substitutions. Most of the bands are observed to be medium, weak and very weak in intensity.

3.2.5 Other Vibrations

In the present case, C=C stretching vibration with weak intensity at 1879 cm^{-1}, CH_2 wagging vibrations with very weak & medium intensity at 940 and 901 cm^{-1} respectively, C-C=O bending vibration with weak intensity at 569 & 550 cm^{-1}, O=C=O bending vibrations with very strong and medium intensity at 350 and 330 cm^{-1} respectively, O-K stretching vibration with very strong intensity at 260 & 200 cm^{-1}, O-K stretching vibrations with medium intensity at 180 & 150 cm^{-1} and O-K stretching vibration with weak intensity at 110 cm^{-1} are observed.

3.3 Powder X–Ray Diffraction Studies

The powder X-ray diffraction pattern for L-Glutamine potassium carbonate crystal is compared with joint committee of powder diffraction standard card. It is seen with well defined peaks and are acknowledged from Figure (5) confirming the presence of potassium carbonate

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and presence of L-Glutamine amino acid group. The observed peaks are in good agreement with the data. The sharp peaks confirm the purity and crystallinity of the title compound material.

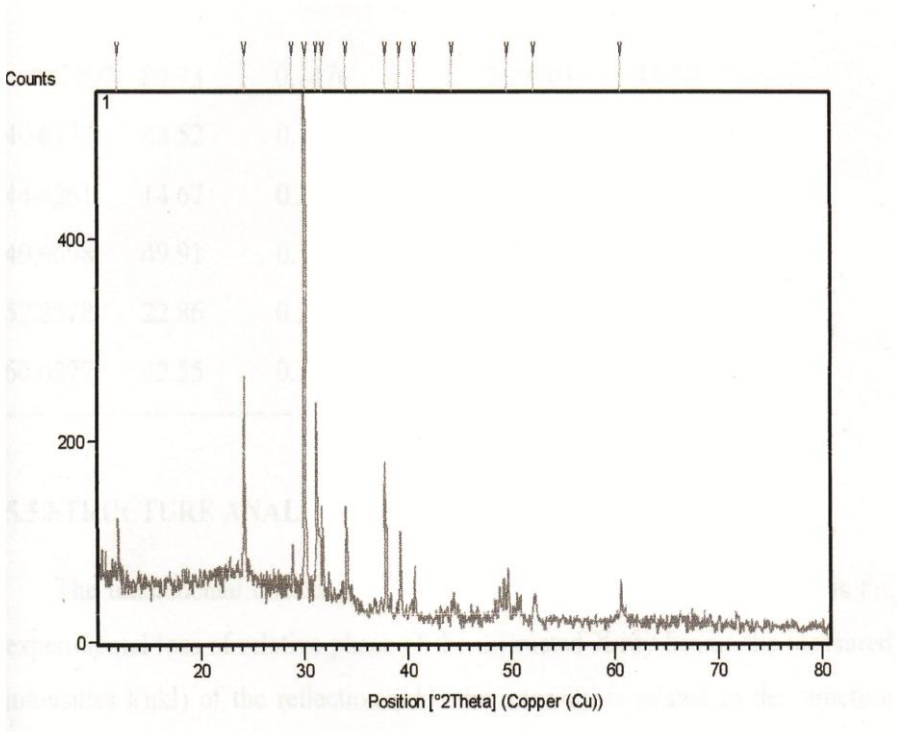

Figure 5: Powder XRD pattern of L-Glutamine Potassium Carbonate Crystals

3.4 UV-Visible Spectral Studies

The optical absorption spectra of L-Glutamine potassium carbonate crystal were recorded in the region 200 to 1100 nm at a scanning speed of 480 nm/min. Figure [6 (a & b)] shows that the absorbance and transmission spectra which holds good in the entire visible region. The Glutamine with potassium carbonate crystal has good transmittance and the lower cut off wavelength is observed at 208.03 nm. The large transmittance in the entire visible region enables it to be a good candidate for optoelectronic applications.

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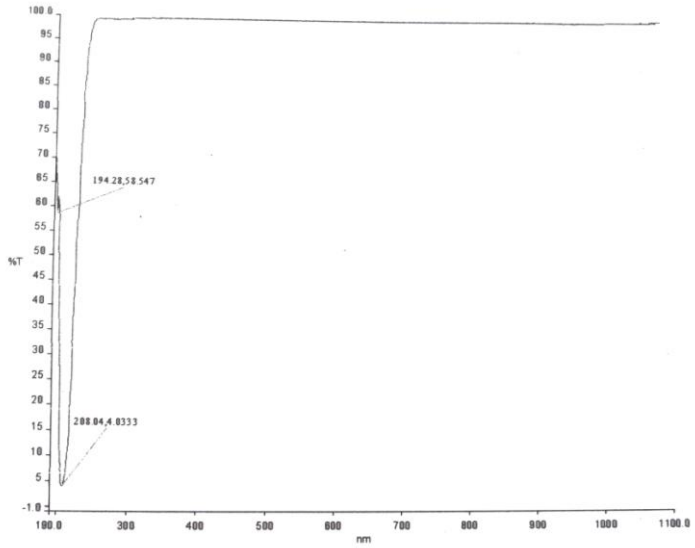

Figure 6: (a) Transmission spectra of L-Glutamine Potassium Carbonate Crystals

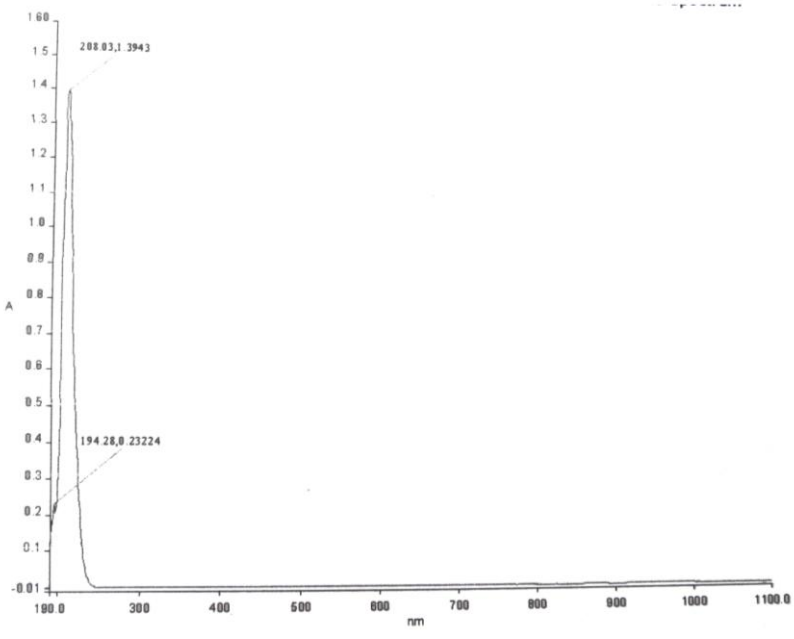

Figure 6: (b) Absorption spectra of L-Glutamine Potassium Carbonate Crystals

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3.5 Mechanical Studies

The micro hardness of a substance is an important property to expose the strength of the material which is basically related to the crystal structure and about the atomic package. It also reveals the electronic factors operating to make the stable structure. Hardness is normally defined as the resistance offered by the crystal for the movement of dislocations and for localized plastic deformation. This test affords useful details about the mechanical properties like elastic constants, yield strength, etc. of materials. The variations of H_v with the applied load for the L-Glutamine potassium carbonate crystals are shown in Figure (7). The hardness number was found to increase with increase in applied load, which confirms the hardness. The micro hardness test conducted on the experimental crystal proves its greater physical strength. Micro hardness studies are well explained by the increase in hardness value with increase in Load and shown in Table (4).

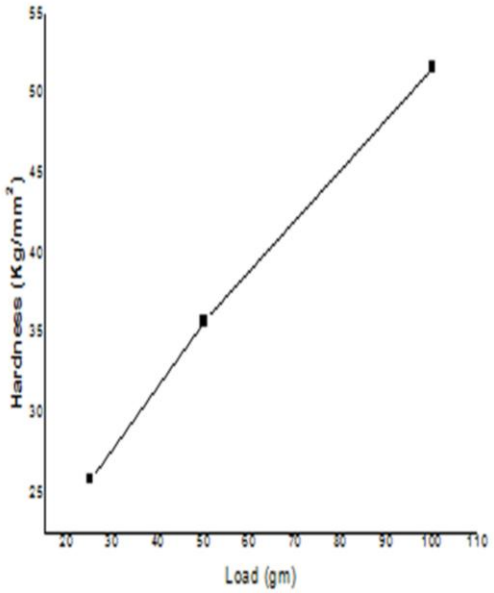

Figure 7: Variation of Hardness with Load of L-Glutamine Potassium Carbonate Crystals

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Table (4): Microhardness of L-Glutamine Potassium Carbonate crystals

S. No.	Load (grams)	(H_V)
1	25	25.8
2	50	35.7
3	100	51.5

4. Conclusion

Single crystal of L-Glutamine Potassium Carbonate, a new semi organic non-linear optical crystal has been grown by slow evaporation technique. The FT-IR and FT-Raman spectra were recorded and the detailed vibrational assignments using HF and DFT methods. The difference between the corresponding wave numbers (observed and calculated) is very small for most of the fundamentals. Therefore, the results presented in this work for L-Glutamine Potassium Carbonate indicate that this level of theory is reliable for the prediction of both Infrared and Raman spectra of the title compound. FT-IR and FT-Raman spectrum reveals the functional groups of the grown title compound material are upto anticipation. Powder X ray diffraction method confirmed the presence of atoms and purity of the material. The crystal has good optical character in the entire UV-Visible region. The micro hardness test confirms the mechanical strength of the crystal. Further this new semi organic non-linear optical material may be considered for optoelectronic and other photonic applications.

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