

VIBRATIONAL WAVENUMBERS AND STRUCTURAL DETERMINATION OF DILITHIUM TEREPHTHALATE

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ABSTRACT

A complete vibrational spectrum analysis of dilithium terephthalate is performed. The normal mode wavenumbers are calculated on the basis of ab initio force fields using Hartree-Fock 6-31G basis set theoretical optimized geometry. Assignments of all vibrational bands have been performed taking into account the results of ab initio vibrational analysis. Predicted infrared, Raman intensities, force constants and depolarization ratios are reported.*

Keywords : *Vibrational wavenumbers, terephthalate, HF ab initio calculations*

INTRODUCTION

Terephthalic acid finds extensive application in the polymer industry. By far the most important use is in the manufacture of synthetic fibres of polyester type (notably dacron and terylene); second in importance is its use as an intermediate for polyester films¹. Understanding the nature of terephthalate complexes of catalyst and corrosion metals will lead to process insights and improvements. The crystal structure of dilithium terephthalate has been solved by ab initio using Monte Carlo simulated annealing techniques, and refined using synchrotron powder data by Kaduk². Li₂C₈H₄O₄ crystallizes in P2₁/c, with a=8.35921, b=5.13208, c=8.48490 Å, V= 363.451 Å³, z=2. The Li anions are tetrahedrally coordinated and the packing of the terephthalate anions resembles the γ -packing of aromatic hydrocarbons². Moskovits and Suh³ and Boerio and Roth⁴ have reported independently the surface enhanced Raman scattering spectra of terephthalic acid, a highly symmetric dicarboxylic acid in aqueous silver sol. Infrared and Raman spectroscopic studies of dipotassium and disilver salts of terephthalic acid were reported by Lee *et al.*⁵. Klug *et al.*⁶ investigated the adsorption of phthalic acid on an oxidized aluminium foil by Raman spectroscopy. Direct characterization of phthalic acid isomers in mixtures using surface enhanced Raman scattering was reported by Bello *et al.*⁷. Tellez *et al.*⁸ reported the Fourier transform infrared and Raman spectra and ab initio calculations of terephthalic acid and related compounds. The IR, Raman, surface enhanced Raman scattering spectra and ab initio calculations of disodium terephthalate are reported by Varghese *et al.*⁹. Ab initio quantum mechanical method is at present widely used for simulating IR spectrum. Such simulations are indispensable tools to perform normal coordinate analysis so that modern vibrational spectroscopy is unimaginable without involving them. In the present study the theoretical calculations of the wavenumbers of the title compound and assignments are reported.

EXPERIMENTAL

0.3093 gm of Li₂O was dissolved in 40 ml of distilled water and 1.6712 gm of terephthalic acid was added to this solution. The resulting solution was filtered to remove a few black specks. To

this clear solution was added 40 ml of ethanol. After evaporating the solvent over two days, a yield of 1.453 gm of white solid was obtained.

Computational Details:

Calculations of the title compound were carried out with Gaussian03 program¹⁰ using the HF/3-21G* basis set to predict the molecular structure and vibrational wavenumbers. Molecular geometry was fully optimized by Berny's optimization algorithm using redundant internal coordinates. Harmonic vibrational wavenumbers were calculated using the analytic second derivatives to confirm the convergence to minima on the potential surface. The wavenumber values computed at the Hartree-Fock level contain known systematic errors due to the negligence of electron correlation¹¹. We therefore, have used the scaling factor value of 0.9085 for HF/3-21G* basis set. Parameters corresponding to optimized geometry of the title compound (Fig.1) are given in Table 1. The absence of imaginary wavenumbers on the calculated vibrational spectrum confirms that the structure deduced corresponds to minimum energy. The assignments of the calculated wavenumbers are aided by the animation option of MOLEKEL program, which gives a visual presentation of the vibrational modes^{12,13}.

RESULTS AND DISCUSSION

The assignments of the benzene ring vibrations of the title compound in Wilson notation¹⁴ is made by referring to the case of benzene derivatives with di-light substituents as summarized by Varsanyi¹⁵, Boeiro and Roth⁴ and Arenas and Marcos^{16,17}

The carboxylate group^{18,19} gives rise to two bands: an asymmetric CO₂ stretching band in the range 1525-1605 cm⁻¹ and a symmetric CO₂ stretching band in the range 1380 -1450 cm⁻¹. When a carboxylic acid changes into a carboxylate the C=O and C-O are replaced by two equivalent carbon-oxygen bonds which is intermediate in force constant between C=O and C-O. The $\nu_{\text{C=O}}$, occurring in carboxylic acid at 1725 cm⁻¹, shifts to a wavenumber lower by ≈ 130 cm⁻¹, and the $\nu_{\text{C-O}}$, occurring at 1250 cm⁻¹, to ≈ 130 cm⁻¹, higher wavenumber to give the CO₂ antisymmetric and symmetric stretching vibrations¹⁸. The $\nu_{\text{as}}\text{COO}^-$ bands are reported to be at 1562 cm⁻¹ (IR) for dipotassium terephthalate and at 1573 cm⁻¹ (IR) and 1516 cm⁻¹ (Raman) for disilver terephthalate⁵. For disodium terephthalate this mode is reported at 1617, 1558 cm⁻¹ (IR), 1599 cm⁻¹ (Raman) and at 1615, 1540 cm⁻¹ theoretically⁹. The symmetric stretching modes of COO⁻ group are reported at 1400 and 1378 cm⁻¹ for dipotassium terephthalate salt⁵, at 1385, 1376 cm⁻¹ for disilver terephthalate salt⁵ and at 1397 (IR), 1403, 1378 cm⁻¹ (HF) for disodium terephthalate salts⁹. For the title compound, the HF calculations give values at 1524, 1485 and 1399, 1396 cm⁻¹ as antisymmetric and symmetric CO₂ stretching modes, respectively.

The δCO_2 vibration is active in the region 795 ± 65 cm⁻¹ and the CO₂ wagging vibration give rise to band with variable intensity in the range 670 ± 30 cm⁻¹¹⁸. Lee *et al.*⁵ reported the bending modes of COO⁻ group at ~ 705 and 744 cm⁻¹ for terephthalate salts. According to Joo *et al.*²⁰ the bending mode of the carboxylate group appear at ~ 830 cm⁻¹ for phthalic acid and at 851 cm⁻¹ for sodium salt of phthalic acid. For disodium terephthalate the bending modes of COO⁻ group are reported at 746 (IR), 712, 688, 629 cm⁻¹ (Raman) and at 755, 708, 679, 620 cm⁻¹ theoretically⁹. In the present case the modes 848, 768, 661, 648 cm⁻¹ are assigned as the bending modes of CO₂ group. The COO⁻ rocking vibration¹⁸ is located in the region 515 ± 65 cm⁻¹ with a weak to medium intensity, well separated from the wagging mode. For disilver terephthalate salt⁵ ρCO_2 is reported at 534 cm⁻¹ and for disodium terephthalate⁹ at 538 (Raman), 508 (IR), 527, 518 cm⁻¹ (HF). The CO₂ torsional modes¹⁸ are expected in the region 195 ± 50 cm⁻¹ and are found in the low wavenumber region.

The phenyl CH stretching occur above 3000 cm^{-1} and is typically exhibited as a multiplicity of weak to moderate bands, compared with the aliphatic C-H stretchings^{18,21}. The calculated values are 3104 , 3101 , 3090 and 3089 cm^{-1} . The benzene ring possesses six ring stretching vibrations, of which the four with the higher wavenumbers (8a, 8b, 19a, 19b occurring, respectively, near 1600 , 1580 , 1490 and 1440 cm^{-1}) are good group vibrations. When the ring is substituted at 1,4-position with identical substituents, both vibrations 8a and 8b are infrared inactive^{15,18}. There is a center of symmetry in benzene ring compounds which have identical groups on all the para pairs of ring carbons. This includes symmetrical para-, symmetrical tetra-, hexasubstituted benzenes and benzene itself. For these types of substitution, the quadrant stretching vibrations are infrared inactive because all the ring atoms para to each other move in exactly opposite directions²². The fifth ring stretching vibration $\nu_{\text{Ph}} 14$ is active near $1315 \pm 65\text{ cm}^{-1}$. The sixth ring stretching vibration or ring breathing mode $\nu_{\text{Ph}} 1$ appears as a weak band near 1000 cm^{-1} in mono, 1,3-di and 1,3,5-trisubstituted benzenes. In the otherwise substituted benzenes, however, this vibration is substituent sensitive and difficult to distinguish from the ring in-plane deformation. As seen from Table 2, the ab initio calculations give wavenumbers at 1629 , 1596 , 1450 , 1430 and 1330 cm^{-1} as ν_{Ph} modes. These vibrations are expected in the region $1280 - 1630\text{ cm}^{-1}$ ¹⁸.

In para disubstitution, the C-X in-plane bending vibrations¹⁵ are expected in the region $260 - 490\text{ cm}^{-1}$ (mode 9b) and $190 - 350\text{ cm}^{-1}$ (mode 15). When the substituents are identical, vibration 9b is active in the Raman spectrum but vibration 15 is Raman inactive¹⁵. For disodium terephthalate⁹, the $\delta_{\text{CX}}(\text{X})$ are reported at 328 , 286 cm^{-1} experimentally and at 323 , 291 , 271 cm^{-1} theoretically. The HF calculations give 382 , 281 , 269 , 207 , 164 and 120 cm^{-1} as the substituent sensitive bending vibrations. In para disubstitution, vibrations 1 and 12 have substituent sensitive wavenumbers¹⁵. When both substituents are light the two vibrations couple with a corresponding C-X stretching vibrations which results in the frequency decrease of both modes. When the substituents are identical, vibration 1 can only appear in the Raman spectrum, while mode 12 is found in the IR spectrum¹⁵. The mode 1 is expected in the region $720 - 860\text{ cm}^{-1}$ and mode 12 in the region $680 - 760\text{ cm}^{-1}$ ¹⁴. Lee *et al.*⁵ reported mode 1 at $\sim 855\text{ cm}^{-1}$ and mode 12 at $\sim 820\text{ cm}^{-1}$ for disilver terephthalate salts. For disodium terephthalate mode 12 is reported at 861 cm^{-1} (Raman), 854 cm^{-1} (HF) and mode 12 at 746 cm^{-1} (IR), 755 cm^{-1} (HF)⁹. In the present case, the ring breathing mode is assigned at 858 cm^{-1} whose IR intensity is zero while the Raman activity is high (Table 2).

In para substitution, normal vibrations 7a and 13 are assigned to the C-X stretching modes when the two substituents are light¹⁵. For identical substituents, the vibration 7a has a higher frequency than that of mode 13, except for p-xylene¹⁵. The substituent sensitive $\nu_{\text{CX}}(\text{X})$ vibrations¹⁸ are expected in the region 1245 ± 50 and $1160 \pm 90\text{ cm}^{-1}$. For disodium terephthalate these substituent sensitive modes are reported at 1185 , 1135 cm^{-1} (Raman) and 1174 , 1126 cm^{-1} by ab initio calculations⁹. The HF calculations give bands at 1192 and 1111 cm^{-1} as $\nu_{\text{CX}}(\text{X})$ modes for dilithium terephthalate. The CH out-of-plane deformations¹⁸ are observed between 1000 and 780 cm^{-1} . Generally C-H out-of-plane deformations with the highest wavenumbers have a weaker intensity than those absorbing at lower wavenumbers. The strong CH out-of-plane deformation occurring at $840 \pm 50\text{ cm}^{-1}$ is typical for 1,4-disubstitution. The lower CH out-of-plane deformations absorb in the same neighbourhood ($820 \pm 45\text{ cm}^{-1}$) but is much weaker or infrared inactive.

According to Kaduk² the Li-O bond distance span in a wide range and the average distance in Li-O coordination sphere is 1.969 \AA . The coordination of each Li is tetrahedral and each oxygen atom is coordinated to two different Li. There is no chelation; the carboxyl groups

bridge lithium cations and soft constraints were applied in the calculation of Kaduk². In the present study, no such coordination is considered and the ab initio calculations give Li-O distance as 1.8462 Å on an average. For the carboxyl group, Kaduk² reported the value $C_{\text{ring}}-C_{\text{carboxyl}} = 1.481$ Å and the C-O distances as 1.271 Å, subject to self constraints. In the present study, the above values are 1.48 and 1.275 Å, respectively. For the title compound, the reported values of O-C-O and C-C-O angles are 123.8 and 119.6°¹ whereas the present calculation (without any constraints) give the values as 118.8 and 120.6°. In the vibrational analysis of terephthalate ions Boeiro *et al.*⁴ reported, the lengths of the CC and CH bonds in the benzene ring and CC bond length between the ring and the carboxylate group are 1.397, 1.084 and 1.51 Å, respectively. The CO bond length is reported as 1.20 Å [4]. The X-ray diffraction results for the terephthalate acid gave a CCO angle of 117.3° and CC, CO bond lengths as 1.37 and 1.27 Å, respectively⁸. In the present study, these values are 120.6°, 1.3801 Å and 1.2753 Å, respectively. These differences can be explained by means of the associated terephthalate acid molecules in the solid state, which tend to stretch out the molecule in a long chain forming the crystalline net. All the carbon-carbon bond lengths in the benzene ring lie in the range 1.3801 – 1.3846 Å and C-H bond length is 1.0695 Å. Here for the title compound, benzene ring is a regular hexagon with bond lengths somewhere in between the normal values for a single (1.54 Å) and a double (1.33 Å) bond²³.

Table-1: Optimized geometrical parameters of dilithium terephthalate, atom labeling is according to Fig. 1

Bond lengths (Å)		Bond angles (°)		Dihedral angles (°)	
C ₁ -C ₂	1.3801	A(2,1,6)	119.5	D(6,1,2,3)	-0.0
C ₁ -C ₆	1.3846	A(2,1,7)	121.6	D(6,1,2,8)	-180.0
C ₁ -H ₇	1.0695	A(6,1,7)	118.9	D(7,1,2,3)	180.0
C ₂ -C ₃	1.3846	A(1,2,3)	119.5	D(7,1,2,8)	-0.0
C ₂ -H ₈	1.0695	A(1,2,8)	121.6	D(2,1,6,5)	0.0
C ₃ -C ₄	1.3846	A(3,2,8)	118.9	D(2,1,6,12)	-180.0
C ₃ -C ₁₁	1.4796	A(2,3,4)	121.0	D(7,1,6,5)	-180.0
C ₄ -C ₅	1.3801	A(2,3,11)	119.5	D(7,1,6,12)	0.0
C ₄ -H ₉	1.0695	A(4,3,11)	119.5	D(1,2,3,4)	-0.0
C ₅ -C ₆	1.3846	A(3,4,5)	119.5	D(1,2,3,11)	180.0
C ₅ -H ₁₀	1.0695	A(3,4,9)	118.9	D(8,2,3,4)	180.0
C ₆ -C ₁₂	1.4795	A(5,4,9)	121.6	D(8,2,3,11)	-0.0
C ₁₁ -O ₁₃	1.2753	A(4,5,6)	119.5	D(2,3,4,5)	0.0
C ₁₁ -O ₁₄	1.2753	A(4,5,10)	121.6	D(2,3,4,9)	-180.0
C ₁₁ -Li ₁₇	2.1337	A(6,5,10)	118.9	D(11,3,4,5)	-180.0
C ₁₂ -O ₁₅	1.2753	A(1,6,5)	121.0	D(11,3,4,9)	0.0
C ₁₂ -O ₁₆	1.2753	A(1,6,12)	119.5	D(2,3,11,13)	-179.9
C ₁₂ -Li ₁₈	2.134	A(5,6,12)	119.5	D(2,3,11,14)	-0.0
O ₁₃ -Li ₁₇	1.8461	A(3,11,13)	120.6	D(4,3,11,13)	0.0
O ₁₄ -Li ₁₇	1.846	A(3,11,14)	120.6	D(4,3,11,14)	179.9
O ₁₅ -Li ₁₈	1.8463	A(13,11,14)	118.8	D(3,4,5,6)	-0.0
O ₁₆ -Li ₁₈	1.8463	A(6,12,15)	120.6	D(3,4,5,10)	-180.0
		A(6,12,16)	120.6	D(9,4,5,6)	180.0
		A(15,12,16)	118.8	D(9,4,5,10)	-0.0

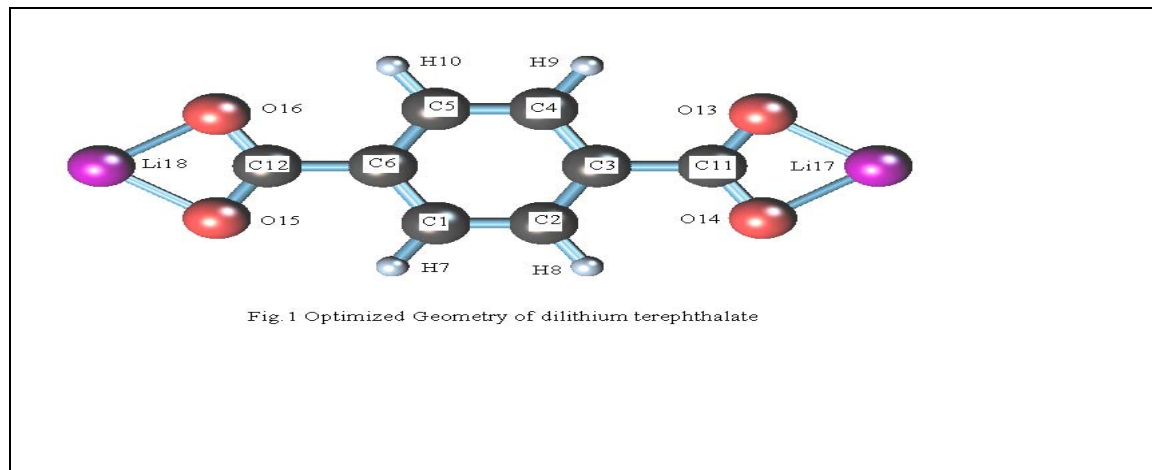
A(13,17,14)	73.0	D(4,5,6,1)	-0.0
A(15,18,16)	72.9	D(4,5,6,12)	180.0
L(3,11,17,4,-1)	180.0	D(10,5,6,1)	180.0
L(6,12,18,1,-1)	180.0	D(10,5,6,12)	-0.0
L(3,11,17,4,-2)	179.5	D(1,6,12,15)	0.0
L(6,12,18,1,-2)	179.8	D(1,6,12,16)	180.0
		D(5,6,12,15)	-180.0
		D(5,6,12,16)	-0.0

Table-2: Calculated wavenumbers and band assignments for dilithium terephthalate

$\nu_{(\text{HF})}$ (cm^{-1})	IR Intensity (KM/mole)	Raman activity ($\text{\AA}^4/\text{amu}$)	Force constants (mDyne/\AA)	Depolarization ratio (P)	Depolarization ratio (U)	Assignments
3104	0.00	172.16	7.54	0.16	0.28	ν_{CH} 20a
3101	0.31	0.00	7.51	0.65	0.79	ν_{CH} 20b
3090	0.00	75.62	7.41	0.75	0.86	ν_{CH} 2
3089	0.06	0.00	7.42	0.59	0.74	ν_{CH} 7b
1629	0.00	224.18	9.78	0.42	0.59	ν_{Ph} 8a
1596	0.00	1.22	12.80	0.75	0.86	ν_{Ph} 8b
1524	39.87	0.00	3.96	0.62	0.79	ν_{asCO_2}
1485	754.66	0.00	14.08	0.42	0.59	ν_{asCO_2}
1450	0.00	1.80	16.08	0.75	0.86	ν_{Ph} 19a
1430	0.01	123.63	17.33	0.19	0.33	ν_{Ph} 19b
1399	1287.75	0.00	9.19	0.36	0.53	ν_{sCO_2}
1396	87.44	0.00	3.61	0.20	0.33	ν_{sCO_2}
1330	0.00	0.22	1.66	0.75	0.86	ν_{Ph} 14
1204	93.58	0.00	6.12	0.32	0.48	δ_{CH} 13
1192	0.00	10.47	1.20	0.12	0.22	$\nu_{\text{CX(X)}}$ 7a
1143	8.50	0.00	3.52	0.38	0.56	δ_{CH} 9a
1111	0.00	16.99	7.06	0.15	0.26	$\nu_{\text{CX(X)}}$ 13
1095	0.56	0.00	1.44	0.58	0.74	δ_{CH}
1089	0.00	5.29	1.30	0.75	0.86	δ_{CH}

1086	0.00	0.00	1.18	0.69	0.82	ν C-C
1037	12.04	0.00	1.99	0.747	0.85	ν C-C
954	16.11	0.00	1.24	0.18	0.30	γ CH 17a
925	0.00	2.48	0.76	0.75	0.86	γ CH 10b
858	0.00	48.99	5.55	0.01	0.16	Ring breathing 1
848	0.02	8.31	2.31	0.75	0.86	δ CO ₂
842	76.29	0.00	6.02	0.73	0.84	γ CH 10a
768	223.19	0.00	1.33	0.02	0.05	δ CO ₂ 12
742	0.00	2.23	3.28	0.12	0.21	γ CH 4
717	0.00	1.44	1.64	0.75	0.86	γ Ph
661	0.00	7.570	2.22	0.75	0.86	ω CO ₂
648	580.17	0.00	2.40	0.54	0.69	ω CO ₂
633	0.05	1.08	2.21	0.40	0.59	δ Ph 6b
536	0.00	0.04	1.37	0.75	0.86	ρ CO ₂
496	0.10	0.00	2.06	0.74	0.85	ρ CO ₂
485	1.68	0.00	0.63	0.32	0.49	γ Ph(X)
468	11.49	0.00	1.14	0.50	0.67	δ Ph(X)
449	0.00	0.00	0.40	0.72	0.84	δ Ph(X)
413	0.00	0.06	0.91	0.75	0.86	γ Ph 16a
382	64.94	0.00	0.91	0.75	0.86	γ CX(X) 5
281	0.00	3.47	0.44	0.75	0.86	δ CX(X) 9b
269	0.00	3.37	0.62	0.27	0.42	δ CX(X) 9b
207	0.00	0.49	0.20	0.75	0.86	γ CX(X)
164	169.33	0.00	0.17	0.61	0.76	τ CO ₂ 15
120	0.00	0.00	0.08	0.75	0.86	τ CO ₂ 15
118	11.90	0.00	0.09	0.75	0.86	τ Ph
110	0.00	1.26	0.06	0.75	0.86	τ Ph
76	0.00	0.00	0.06	0.75	0.86	τ Ph(X)
63	29.63	0.00	0.02	0.72	0.84	τ Ph(X)

ν , stretching; δ , in-plane deformation; γ , out-of-plane deformation; ρ , rocking; ω , wagging; τ , torsional; Ph, phenyl; X, substituent sensitive;



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