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Vibrational Analysis of 5'-Methyl-6b,7,9,11a-tetrahydrospiro [chromeno [3', 4': 3,4] pyrrolo [1,2-] thiazole-11,3'-indoline]-2',6(6a*H*)-dione

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ABSTRACT

Single Crystal of 5'-Methyl-6b,7,9,11a- tetrahydrospiro [chromeno [3', 4': 3,4] pyrrolo [1,2-c] thiazole-11,3'-indoline] -2', 6 (6aH) -Dione was grown and from single crystal XRD, the lattice parameters are a = 8.365Å, b = 9.765 Å, c = 11.968Å, α= 112.62°, β = 99.39°, γ = 91.89°and it belongs to Triclinic space group P-1. The compound was characterized by FT-IR and Raman analyses. The presence of different functional groups and the nature of their vibrations were identified in experimental vibrational studies through Infra-red and Raman measurements in the range of 4000-400 cm^{-1}.

Keywords: FTIR Spectrum, Indoline, Pyrrole, Raman Spectrum, Thiazole.

I. INTRODUCTION

Pyrrole derivatives are well known in many marine organisms [1], some show important bioactivities, such as antitumor activity [2], protein kinase inhibiting activity [3], precursors in porphyrin synthesis [4, 5] and as monomers in polymer chemistry [6], with applications ranging from nonlinear optical materials [7] to electronic noses [8], as selective glycosidase inhibitors, which are used in the treatment of diabetes, cancer, malaria and viral infections, including AIDS [9].

Thiazole and its derivatives are of significant importance in medicinal chemistry as bacterial, herbicidal, fungicidal, antitumor agents [10]. Thiazole derivatives have been used in pharmacological applications, such as antifungal, antiviral, antibacterial, anticancer and anti-inflammatory activities [11]. Thiazole derivatives exhibit diverse biological activities as bacteriostatic, antituberculous and fungistatic agents [12].

Indole derivatives posses biological properties such as antitumor [13], antibacterial and fungicidal [14], anticancer and anti-HIV [15] activities.

Fig.1

II. VIBRATIONAL ANALYSIS

The title compound [C_{21} H_{18} N_2 O_3S] belongs to the space group P-1and has a triclinic symmetry with two formula units per cell. The factor group analysis using the standard correlation method was carried out. Excluding the acoustic modes, 267 normal modes are predicted. These genuine modes can be decomposed into the irreducible representations of the factor group $C_i$as $\Gamma = 135A_g^{R}+132A_u^{IR}$ (Table 1), where A_g species are Raman active and A_u species are infrared active. The observed infrared spectrum of the title compound in the spectral range between 4000 and 400 $cm^{-1}$is presented in Fig.2 and the corresponding Raman spectrum in the spectral range between 4000 and 70 cm^{-1} is depicted in Fig.3 The observed vibrational bands in the infrared and Raman spectra with their corresponding assignments are tabulated in Table 2. The molecular structure has various functional groups such as carbonyl, hydroxyl, CH_3, CH2, C-H, C-C=O, C-N, C=O, N-H, C-S and monosubstituted benzene ring. The high wavenumber region around 3800-1500cm^{-1} consists the bands due to N-H, O-H, CH, CH_2 and C-N stretching vibrations. The low wavenumber region around 1500-450 cm^{-1} contains bands due to deformation vibrations of the various groups. The lattice vibration modes occur below 450 cm^{-1}.

Table 1

Factor group analysis of the title compound, $C_{21}H_{18}N_2O_3S$
Crystal space group: P-1 = $C_i^{;}$ Z=2; Z^B =2

	Degreesof freedom for each species	Molecular symmetry species	Modes and Site symmetry species C_1	Factor group species C_i
$C_{21}H_{18}N_2O_3S$	Vibrational 270		A	$135A_g$ $132A_u$

$$\Gamma_{cryst}^{total} = 135A_g^{R} + 135A_u^{IR}$$
$$\Gamma_{cryst}^{int} = \Gamma_{cryst}^{total} - \Gamma^{acoustic} = 135A_g + 135A_u - (3A_u)$$
$$\Gamma_{cryst}^{int} = 135A_g^{R} + 132A_u^{IR}$$

The notation proposed by Wilson[12] will be used throughout this paper for assigning the wavenumbers to the vibrational bands in the spectra.

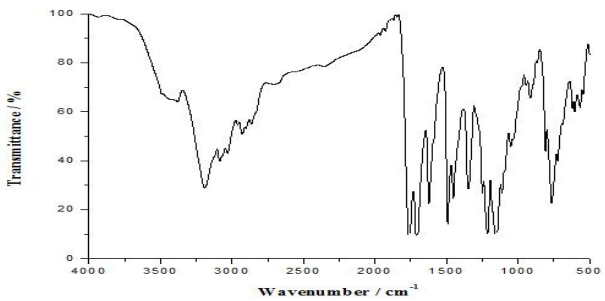

Fig.2 Infra-red spectrum

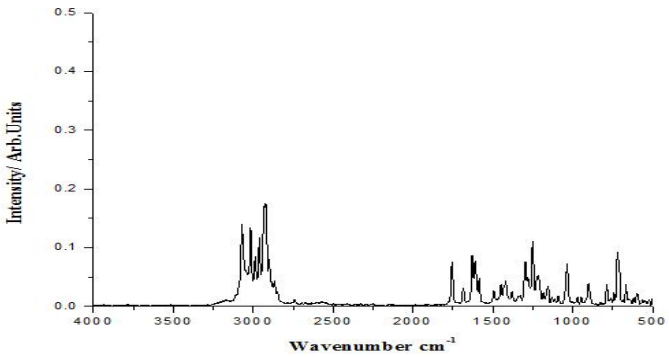

Fig3. Raman spectrum

2.1 Monosubstituted Benzene Ring Vibrations

The wave numbers of the aromatic C-H stretching vibrations in monosubstituted benzenes fall in the range 3100 - 3000 cm^{-1} [33,35,36,44,45]. In the infrared spectrum one medium band at 3086 and one weak band at 3030cm^{-1}, whereas in the Raman Spectrum two strong bands at 3070 and 3017 cm^{-1} are assigned to aromatic C-H stretching vibrations.

In the substituted benzenes, the vibrations in the region 1600 – 1500 cm^{-1} mainly involve quadrant stretching of the ring C=C bonds. But there is a little interaction with CH in plane bending [33, 42]. In the present investigation, the strong band at 1490 cm^{-1}in FTIR, the bands at 1493 $cm^{-1,}$1586$cm^{-1}$and 1612cm^{-1}inRaman spectra are due to quadrant ring stretching components.

The Semi-circle ring stretching vibrations mix strongly with C-H in–plane bending vibrations and split into two components (υ_{19a} and υ_{19b}) in substituted benzenes. The first component (υ_{19a}), involving Semi-circle ring stretching mixed with C-H bending, usually appears at 1510- 1470cm^{-1} for monosubstituted benzenes [33, 42]. The infrared intensity is strong for electron donor groups and weak or absent when these are not present. The Raman intensity is usually weak. In the crystal under study, this mode appears as a strong band at 1490 cm^{-1}in FTIR and a weak band (1493cm^{-1}) in the Raman spectrum. The second component involving semi circle stretching mixed with C-H bending appears at 1465 – 1430 cm^{-1} for monosubstituted benzenes [33, 42]. The infrared intensity of this component is relatively independent of the nature of the substituent. The Raman intensity is usually weak. The strong band at 1452cm^{-1} in the infrared spectrum and the corresponding weak intensity Raman bands at 1451 cm^{-1}, 1419 $cm^{-1}$are due to this component.

In-plane C-H deformation mode (υ_{18b}) falls in the range 1082-1065$cm^{-1}$and is very weak in intensity in both the infrared and Raman spectra [33, 43]. In the present investigation, the weak bands at 1051cm^{-1} in FTIRand at 1091cm^{-1} in Raman spectrum are assigned to in-plane C-H deformation mode (υ_{18b}).

In monosubstituted benzene, a Raman band of medium intensity at 1160 - 1150cm^{-1} appears due to the in-plane C-H deformation mode (υ_{15}) [33,43]. A medium intensity Raman band at 1155cm^{-1} is attributed to the in-plane C-H deformation υ_{15} mode. As this mode is overlapped by C-N-H stretching and C-S stretching vibrations, the corresponding band in the infrared spectrum appears strong at 1153cm^{-1}. Another in-plane C-H deformation mode (υ_3) is expected to appear in the region 1330-1250cm^{-1} and is very weak in both infrared and Raman

spectra in monosubstituted benzenes [33, 43]. For the compound under study, the weak band at 1248cm^{-1} in the infrared spectrum and the corresponding band at 1251cm^{-1}in Raman spectrum appears as a very strong band instead of a very weak band due to the overlapping of in-plane C-H deformation vibrations are attributed υ_3 mode.

For monosubstituted benzene, the out-of –plane quadrant deformation mode (υ_{16a}) is either forbidden or very weak in the infrared spectrum and is also a very weak band in the Raman spectrum at 420-390cm^{-1} [33,43]. This mode υ_{16a} is forbidden in both infrared and Raman spectra. The other quadrant deformation mode (υ_{16b}) generally occurs in the range 560-430cm^{-1} and is weak in the Raman spectrum. This mode is observed as a strong band at 488cm^{-1} in the infrared spectrum and as a weak band at 499cm^{-1} in the Raman spectrum.

For monosubstituted benzene, the out-of-plane C-H deformation mode (υ_5) gives rise to a Raman band of sufficient intensity. This mode usually occurs in the region 1000-970cm^{-1} and appears as a shoulder on the low wavenumber side of the intense band at 1000cm^{-1} due to the trigonal ring 'breathing' mode (υ_{12}) [43]. The weak intensity band at 970cm^{-1} in the Raman spectrum are assigned to out – of-plane C-H deformation mode (υ_5).

The in-phase, out-of-plane aromatic C-H wag vibrations give rise to strong infrared bands and they appear in the spectrum in different regions according to the number of adjacent hydrogen atoms in the benzene ring. For monosubstituted benzenes, with five or four adjacent hydrogen atoms in this band falls in the region 805-728cm^{-1} [33, 42]. The strong band at765cm^{-1} in the infrared spectrum and the corresponding weak Raman band at 742cm^{-1} are attributed to the in-phase, out-of-plane aromatic C-H wag vibrations.

2.2 Pyrrole Ring Vibrations

In the present investigation, the C-H stretching vibrations of pyrrole ring occur as a strong,broad band at 3188cm^{-1} in the infrared spectrum. Due to the overlapping of C-H stretching vibrations of the pyrrole ring with the N-H stretching vibrations of thiazole ring, a broad band instead of the sharp peak appears in the infrared spectrum [42]. Symmetric stretching vibrations (pyr. half –ring) in the pyrrole ring appears at 1347 cm^{-1} and 1382 cm^{-1} [41] in the infrared and Raman spectrum respectively. Stretching vibrations (pyr. quarter-ring) are attributed at 1329cm^{-1} [41] in the Raman spectrum. Absorbance at 1111 cm^{-1} and 1051 cm^{-1} [41] in the infrared spectrum and corresponding absorbance at 1091 cm^{-1} [41] in the Raman spectrum is attributed to stretching vibrations (pyr. breathing) of the pyrrolering. N-H wagging mode of pyrrole is observed at 765 cm^{-1} and 788 cm^{-1} [37,39] in the infrared and Raman spectrum respectively. The weak intensity band at 619cm^{-1} in the Raman spectrum is assigned to out- of- plane deformation of pyrrole rings [41]

2.3. Carbonyl Vibrations

For the crystal under study, the weak band at 3378 cm^{-1} in the FTIR spectrum is assigned to C=O overtone [44].A very strong band at 1760cm^{-1}in the infrared and a strong band at 1756 cm^{-1} in the Raman spectrum[16,38,42] are assigned to C=O stretching vibrations in Five membered rings.Stretching vibrations of C=O in the six membered rings are observed as a very strong band at 1707 cm^{-1} in FTIR and medium intensity band at 1685 cm^{-1} in the Raman spectrum[16,38,45].Intramolecular hydrogen bonded C=O stretching appears as strong bands at 1622 cm^{-1} and 1630 cm^{-1} in the FTIR and Raman spectrum [44]respectively. The C=O in-plane bending and the out-of-plane bending vibrations are expected in the regions 725±70 cm^{-1} and 540±80 cm^{-1}

[1]respectively [17].In the title compound, the in–plane bending vibrations are identified at 765 cm^{-1}in the FTIR and at 722 cm^{-1} in the Raman spectrum. The out-of-plane bending vibrations are observed at 488 cm^{-1}in the FTIR and the corresponding band at 499 cm^{-1} in the Raman spectrum. The in-plane out-of-phase C=O vibrations are observed at 369 cm^{-1} in the Raman spectrum [16].

2.4. Thiazole Ring Vibrations

In the title compound, the N-H stretching vibrations appear as strong band at 3188 cm^{-1} in the FTIR spectrum [20,31].The medium intensity band at 3086 cm^{-1} and the weak band at in the FTIR are attributed to C-H stretching vibrations of the thiazole ring[22,31].The N-H bending vibrations occur as a very strong band at 1490 cm^{-1} in the FTIR and the weak band at 1493 cm^{-1} in the Raman spectrum[22].The strong band at 1452 cm^{-1} in the FTIR and the corresponding weak band at 1451 cm^{-1} are identified as C-C_{phenyl} bending vibrations[22].Due to the overlapping of C-N-H and C-S stretching vibrations ,a very strong broad band appears at 1153 cm^{-1} in the FTIR and the corresponding weak band at 1155 cm^{-1} in the Raman spectrum[22].The weak bands at 942 cm^{-1} and 947 cm^{-1} in the FTIR and Raman spectrum respectively are identified as N-H wagging[22].The C-S stretching vibrations occur at 619 cm^{-1} in both FTIR and Raman spectrum[23].The weak band at 545 cm^{-1} is assigned to in-plane C-S-C bending[23].

2.5. Indole Ring Vibrations

In the present investigation, the bands at 1452 cm^{-1}, 1248 cm^{-1} ,1111 cm^{-1} are attributed to in-plane N-H bending vibrations [28,29,30]. The out-of-plane C-H bending occurs at 942 cm^{-1} in the FTIR and at 947 cm^{-1} in the Raman spectrum [29]. The band at 619 cm^{-1} in both FTIR and Raman spectrum are assigned to out-of-plane N-H bending vibrations [29]. The out-of-plane N-H bending vibrations appear at 565 cm^{-1} , 545 cm^{-1} in the FTIR and at 563 cm^{-1} in the Raman spectrum [28,29].

2.6. CH_3 Vibrations

For the crystal under study, the weak band at 2960 cm^{-1} and the medium band at 2928 cm^{-1} in the FTIR and the corresponding strong bands at 2963 cm^{-1} and 2922 cm^{-1} are observed as antisymmetric (CH3) stretching vibrations [16].The symmetric C-H vibrations (CH_3) are identified at 2864 cm^{-1} in the FTIR and at 2868 cm^{-1} and 2741 cm^{-1} in the Raman spectrum[16].The strong band at 1452 cm^{-1} and the corresponding weak band at 1451 cm^{-1}in the FTIR and the weak band at 1382 cm^{-1} are assigned to antisymmetric deformation of CH_3[16]. CH_3 rocking appears at 1051 cm^{-1}in the FTIR and 1091 cm^{-1} in the Raman spectrum [16].

2.7. CH_2 Vibrations

The medium intensity band at 3086 cm^{-1} and weak band at 3030 cm^{-1}in the IR and the corresponding strong bands at 3070 and 3017cm^{-1} in the Raman indicate the presence of the CH_2 asymmetric stretching vibration [16, 34, 38, 39, 41, 42]. The CH2 symmetric stretching vibration appears as a weak band at 2960cm^{-1} and the medium intensity band at 2928cm^{-1} in the IR and strong bands at 2963 cm^{-1} and 2922 cm^{-1} in the Raman spectrum. The strong peak at 1452$cm^{-1}$and the weak band at 1451 cm^{-1} [34, 42] in the infrared and Raman spectra respectively are attributed to the CH_2 deformation vibrations. The CH_2 twisting vibrations in CH_2 chains

occur at 1051 cm^{-1} in the FTIR and at1329cm^{-1} in the Raman spectrum. The CH_2scissoring, wag and twist vibrations have also been identified and assigned.

2.8. C-N Vibrations

In the title compound, the bands at 1347cm^{-1}, 1213cm^{-1},1111 cm^{-1} and at 1216 cm^{-1} ,1091 cm^{-1} ,1035 cm^{-1} are attributed to C-N stretching vibrations in the infrared and Raman spectrum [26,34,35,44] respectively. The weak intensity bands at 354 and 369 cm^{-1} in the Raman spectrum are assigned to C-N-C skeletal deformations [43].

Table 2

Infrared ($\bar{\upsilon}$ /cm^{-1})	Raman ($\bar{\upsilon}$ /cm^{-1})	Assignment
3378 (w)		νC=O overtone
3188 (s, br)		$\nu N\text{-}H_{thiazole}+\nu C\text{-}H_{pyrrole}$
3086 (m)	3070(vs)	$\nu C\text{-}H_{thiazole}$ + ν_{as}C-H of CH_2 + ν C-H $_{\varphi}$ +ar C-H ν
3030 (w)	3017 (vs)	$\nu_s C\text{-}H_{thiazole}+\nu_{as}$ C-H of CH_2 + ν C-H $_{\varphi}$ +ar C-H ν
2960 (w)	2963 (s)	ν_{as}C-H of $CH_3+\nu_s$C-H of CH_2
2928 (m)	2922 (vs)	ν_{as}C-H of $CH_3+\nu_s$C-H of CH_2
2864 (w)	2868 (w)	ν_sC-H of CH_3
	2741 (w)	ν_sC-H of CH_3
1926		Overtone of indole ring
1760 (vs)	1756 (s)	νC=O Fermi resonance doublet
1707 (vs)	1685 (m)	νC=O
1622 (s)	1630 (s)	C=O intramolecular hydrogen bond+νC-C $_{\varphi}$ + δN-H
	1612 (s)	δN-H+ ν quad.ring
	1586 (m)	ν quad. ring
1490 (vs)	1493 (w)	δ_{as}C-H of CH_3+N-$H_{thiazole}$ bend+ α CH_2+ ν s.c.ring(υ_{19a})+ ν quad.ring
1452 (s)	1451 (w)	α CH_2+ def of CH_3+C-C $_{\varphi}$ bend + Indole skeletal vibrations+ δ N-H+ αCH_3+ ν s.c.ring(υ_{19b})
	1419 (w)	ν s.c.ring(υ_{19b})
	1382 (w)	as .def. of $CH_3+\nu_s$ (pyr.half-ring)
1347 (s, br)		ω CH_2+νC-N+α$CH_3+\nu_s$ (pyr.half-ring)
	1329 (w)	τCH_2+ν (pyr.quarter-ring)+ φ δ CH def. (υ_3)
	1298 (s)	ω CH_2
1248 (w)	1251 (vs)	δ C-H+ φ δ CH def. (υ_3)
1213 (vs, br)	1216 (m)	δ C-H +ν C-N
1153 (vs, br)	1155 (m)	δ C-H + ν C-N-H +νC-S+φ δ CH def. (υ_{15})
1111 (w)		r CH_3+ δ C-H + ν C-N +N-H bending+ ν (pyr.breathing)
	1091 (w)	r CH_3+ δ C-H + ν C-N +N-H bending+ ν (pyr.breathing)+φ δ CH def. (υ_{18b})S
1051 (w)		τ CH_2+ r CH_3 + δ C-H+ + ν C-N+ ν (pyr.breathing)$_+$ φ δ CH def. (υ_{18b})
	1035 (s)	ν C-N
	970 (w)	φ π CH def. (υ_5)
942 (w)	947 (w)	πC-H+ωN-H+indole skeletal vibrations + π C-H
914 (m)	901 (m)	π C-H +r CH
807 (m)		π C-H + δ C-H+ π=CH+ ar CH+ νS-C
	788 (m)	Pyr. N-H ω
765 (s, br)		δ C-C-C + δ C-H+ π indol phenyl ring +In –phase π

		CH(ring) ω+pyr.N-H ω+, δ C=O
	742 (w)	In –phase π CH (ring) ω
722 (w)	722 (vs)	r CH_2 + δ C-C-C+ indole skeletal vibrations+ δO-C-O+ ν S-C-N + δ C=O
619 (w)	619 (w)	ν C-S + δ S-C-N + π N-H + π pyr.def. φ o.p. Sextant ring def. (υ_4)
565 (m)	563 (w)	π N-H+ π S-C-N o.p.def.ofpyr
545 (w)		δ C-S-C + π N-H+ π S-C-N
	499 (w)	φ π quad. def. (υ_{16b}) +π C=O
488 (s)		π N-H+ C-N-C skeletal def.+Carbonyl π def.+ φ π quad. def. (υ_{16b}) +π C=O
	431 (vs)	i.p.C-C(=O)-C def.
	369 (w)	π CCC+C-N-C skeletal def.
	354 (w)	δC=O+ C-N-C skeletal def.
	332 (w)	δCCC+ Torsion C-C
	283 (s)	αCH_2+ Torsion C-C
	225 (m)	Torsion CH_3
	195 (vs)	δCCO
	160 (w)	πCNCH
	118 (vs)	πCNCH
	97 (vs)	Torsion C-C
	83 (vs)	Torsion C-C

ar - aromatic, ν - stretching, as- antisymmetric stretching, s - symmetric stretching, def. - deformation, δ – bending in-plane, π – bending out-of-plane, quad-quadrant, φ - phenyl ring, pyr - pyrrole ring, s.c. - Semi-circle α - scissoring, ω - wagging, τ - twisting, r - rocking.

III CONCLUSION

The compound, 5'-Methyl-6b, 7, 9,11a- tetrahydrospiro [chromeno [3', 4': 3, 4] pyrrolo [1, 2-] thiazole-11,3'-indoline] -2', 6 (6a*H*) -dione was mainly used in biological activities suchas antitumor and anticancer agents. The compound was investigated experimentally by FTIR and Raman vibrational spectroscopic methods. Various functional groups were confirmed by FTIR and Raman spectrum.

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