

Structural Investigation on Curcumin

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Curcumin is non nutrient (phytochemical) extracted from *Curcuma longa* L. (Turmeric). Owing its antitumour and anticancer activities, its importance in the pharmacology field has been escalating. For better understanding on the photobiology of curcumin and its derivatives namely curcuminoids, their spectral, photophysical and photochemical behaviours are to be investigated. This study has been aimed to obtain detailed structural information on the curcumin through its spectral behaviour. For this, a variety of spectra such as UV-Visible, FTIR and NMR have been recorded for the pure curcumin. From the UV-Visible spectral data, different chromophore moieties have been identified for the curcumin molecule. FTIR spectral data gives a wealth of information on the different functional groups of the curcumin molecule. NMR is preeminent technique that has helped in solving the *keto-enolic* tautomerism of curcumin and deciphering the enolic form of the molecule. Also, a host of thermodynamic properties have been obtained for the molecule by molecular mechanics (MM3) methods.

Key Words: Curcumin, UV-Visible spectrum, FTIR spectrum, NMR spectrum, Molecular mechanics.

INTRODUCTION

The use of medicinal plants or their active components in the prevention and treatment of chronic diseases is based on experience from traditional systems of medicine from various ethnic societies. During the past decade, a large number of natural products and dietary components have been evaluated as potential chemo preventive agents¹. Polyphenols, a class of dietary compounds, currently are being evaluated intensively as potential chemopreventive agents². *Curcuma longa* is one of several medicinal plants to have attracted the interest of scientists. Curcumin, natural yellow orange dye extracted

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from the rhizomes of the plant³ *Curcuma longa* L. is thought to have chemopreventive properties. Since, conventional therapy alone has not been fully effective in combating either the high incidence or the low survival rate of several forms of cancer^{4,5} the application of chemopreventive agents to cancer prevention and control has got gained momentum. Besides the pharmacological properties, a host of other properties such as photodynamic agent for the destruction of bacteria⁶, antioxidant property⁷, *etc.* have also been reported. The promising biological properties of curcumin to treat cancer⁸, Alzheimer's disease⁹, HIV^{10,11} chronic inflammations, oxidative stress¹² and cystic fibrosis¹³ have turned the attraction of the scientific community. However, the main hurdle lies in the bioavailability of this molecule. Intense research is also being undertaken to modify the structure of curcumin so as to increase the bioavailability and potency while maintaining the relative non-toxic nature of this natural product¹⁴. This demands for a systematic spectral, photochemical, photophysical investigation and comparative analysis of curcumin and curcuminoids.

EXPERIMENTAL

Pure sample of curcumin was obtained from Asthagiri Herbal Research Foundation, Chennai, India and used without purification. The UV-Visible spectrum of curcumin was scanned in the region between 190-1100 nm using TechComp 8500 model UV-Visible spectrophotometer of spectral width < 2 nm at Asthagiri Herbal Research Foundation Chennai, India. The FTIR spectrum of curcumin was recorded in the region of 4000-400 cm⁻¹ by a Bruker IFS 66V spectrometer of spectral width 2.0 cm⁻¹. The spectral measurements have been carried out at SAIF, IIT, Chennai, India. The NMR studies in the present work have been carried out using Jeol GSX 400 FT NMR instrument at SAIF, IIT, Chennai. It operates at 400 MHz for proton with a magnetic field of 9.3 Tesla. Hence a superconducting magnet is used. Resolution of the instrument is 0.03 Hz for ¹H.

RESULTS AND DISCUSSION

UV-Visible spectra

Curcumin³ and curcuminoids^{6,15} are practically insoluble in water, while soluble in both polar and nonpolar organic solvents. Since curcumin is freely soluble in methanol, the UV-Visible absorption spectrum of curcumin in methanol has been recorded for a random concentration such that the absorbance is in the common useful range. The UV-Visible spectral recording showed four peaks at 192, 205, 254 and 420 nm. The absorption parameters have been given in Table-1.

TABLE-1
UV-VISIBLE ABSORPTION PARAMETERS OF CURCUMIN

Wavelength (nm)	Absorbance
192	0.1183
205	0.2077
254	0.0074
420	0.2437

The absorption of UV-Visible light by organic compounds involves invariably transition of valence electrons. The position of the electronic absorption can be predicted by the chromophore-auxochrome theory. Simple chromophores such as $>C=C<$, $-C=N$ and $-C=C-$ undergo $\pi \rightarrow \pi^*$ transitions in the short wavelength regions of UV radiations. Hence the absorbance peak at 192 nm is due to the $>C=C<$ chromophore. The absorbance peak at 254 nm is due to substituted benzene ring as chromophore¹⁶. Curcumin, in analogy to other β -diketones, is expected to exist in the enol configuration. The absorption peak at 420 nm indicates that the chromophore moieties such as β -diketone, diene, phenyl rings and substituents, *etc.* probably do not act independently but interact strongly with each other due to the conjugation of their π -electrons in the enolic configurations as well as due to the electronic properties of the substituents¹⁷.

Aromatic ring C-C vibrations: Skeletal vibrations, involving carbon to carbon stretching within the ring, absorb in the $1600-1585\text{ cm}^{-1}$ and in the $1500-1400\text{ cm}^{-1}$ region. The skeletal bands frequently appear as doublets, depending upon the nature of the ring substituents¹⁸. For aromatic six membered rings, according to Wilson¹⁹ five normal modes, which belong to this class. The frequencies of these modes are fairly insensitive to substitution. In *para*-substituted benzene ring the intensities of the ring stretching frequencies at $1600-1400\text{ cm}^{-1}$ depend on the charge distribution of the ring²⁰. There are two or three bands in this region due to skeletal vibrations, the strongest being at about 1500 cm^{-1} . In general bands of variable intensity are observed at $1625-1430\text{ cm}^{-1}$. The aromatic ring deformation vibrations occur below 700 cm^{-1} and are quite sensitive to the changes in the nature and position of substituent²¹. The bands at 1509 , 1460 and 1450 cm^{-1} have been assigned to aromatic stretching. The sets of bands 660 , 640 , 620 and 606 cm^{-1} and 572 , 564 , 541 and 512 cm^{-1} have been assigned to aromatic C-C-C out of plane and in-plane deformations, respectively. The stretching and bending vibrational band assignment on the aromatic ring are found to be in good agreement with the literature values.

Aromatic C-H vibrations: Aromatic C-H stretching vibrations occur in the region $3080-3010\text{ cm}^{-1}$ and are off strong to medium intensity. CH in-plane deformation vibrations occur in the region $1290-1000\text{ cm}^{-1}$ usually

being sharp but have weak to medium intensity^{18,22-25}. Bands at 3183 and 2933 cm^{-1} have been assigned to CH stretching vibrations. Bands at 1206, 1185 and 1167 cm^{-1} have been assigned to CH in-plane deformation vibrations which agree well with the value reported by previous work on benzene and its derivatives²⁶⁻²⁹. Since the out of plane deformation vibrations occur below the inplane region, the bands at 1113, 1093 and 1025 cm^{-1} have been assigned to aromatic CH out of plane deformation vibrations.

O-H Vibrations: Hydroxyl groups absorb strongly in the region¹⁸ 3670-3580 cm^{-1} . The in plane O-H deformation vibration gives rise to a strong band in the region 1440-1260 cm^{-1} and the out of plane vibration give a broad band in the region 700-600 cm^{-1} . The bands at 3551 and 1429 cm^{-1} with due characteristics have been assignment to OH stretching and OH in-plane deformation vibrations, respectively.

C=O Stretching vibrations: A great deal of structural information of a molecule can be derived from the exact position of the carbonyl stretching vibrations. If a compound contains a carbonyl group the absorption caused by C=O stretching is generally among the strongest present. C=O stretching vibration is observed in the region 1850-1550 cm^{-1} . Since it occurs as a very strong band and easily recognized. The clear, sharp and strong bands at 1626, 1602 and 1509 cm^{-1} have been assigned to carbonyl stretching vibrations. The assignments are in good agreement with the literature³⁰.

C-O Stretching vibrations: The absorption region for the alcohol C-O group due to its stretching vibration is 1200-1000 cm^{-1} . A strong band and a medium strong band at 1275 and 1233 cm^{-1} , respectively have been assigned to C-O stretching vibrations²⁸.

O-CH₃ Vibrations: Ether vibrations occur in the region of 2995-2840 cm^{-1} and the bands are of medium intensity. Asymmetric CH₃ stretching occurs between 2995-2955 cm^{-1} ; symmetric stretching vibration between 2895-2840 cm^{-1} . Asymmetric and symmetric deformation vibrations of CH₃ occur in the region of 1470-1440 cm^{-1} . Weak bands at 2923 and 2852 cm^{-1} have been assigned to asymmetric and symmetric vibrations of CH₃ group, respectively.

Alkene C=C stretching vibration: Non conjugated alkene have a weak C=C stretching absorption band in the region 1680-1620 cm^{-1} and the band is absent for symmetric molecules. In conjugated system, the C=C stretching vibration frequency is lower than that of an isolated C=C group. A band at 1714 cm^{-1} has been assigned to the C=C stretching vibration.

Alkene C-H vibration: In general, bands due to both alkene and aromatic C-H stretching occur above 3000 cm^{-1} . CH₂ in-plane deformation and scissoring occur in the region 1420-1410 cm^{-1} and the bands generally are of weak intensity. The deformation vibration of C-H may be either perpendicular to or in the plane as that containing the carbon-carbon bonds and the

other bonds. The absorption bands due to the out of plane vibration occur mainly between 1000 and 800 cm^{-1} and have strong to medium intensity. The weak bands at 1373 and 1313 cm^{-1} have been assigned to CH_2 scissoring. The bands at 966 and 961 cm^{-1} have been assigned to alkene CH_2 out of plane bending.

The theoretical vibrational frequencies have been arrived at by performing molecular mechanics computations. The infrared spectral assignments, the experimental and theoretical vibrational frequencies of curcumin have been presented in Table-2.

NMR Spectra

Generally, the NMR signals are reported in chemical shifts termed as δ , which are the ratio of the frequency difference between a reference standard and the test signal to the frequency of the spectrometer. The characteristic chemical shift values have been assigned to different functional units in curcumin molecule based on proton signals obtained from ^1H NMR spectrum are summarized in Table-3 and the results obtained are discussed.

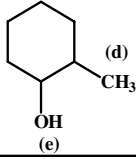
Aliphatic protons: Aliphatic protons, in the absence of any deshielding effects caused by neighbouring groups or atoms are usually the most highly shielded of all the common organic types. Methyl groups in a saturated hydrocarbon environment absorb near 0.9 δ . Acyclic methylene groups (1.25 δ) are less shielded than methyl groups and methine groups (1.5 δ) are still less shielded. This relationship is quite general. Methyl group attached to the aromatic ring through oxygen give a chemical shift between 2.5 and 3.5. Presence of these characteristic peaks confirms the methyl group in the molecule. In β -dicarbonyls the possibility of intramolecular H-bonding can make enol formation much more favourable than ketone form. The chemical shift at 5.7 strongly supports the enolate form of the curcumin molecule. Hence from the ^1H MNR spectrum of curcumin, the molecule is found to exist in the enol form¹⁷.

Aromatic protons: Aromatic protons of substituted benzene generally absorb in the range 6.5-8.5 δ . Electron withdrawing groups³² shift the absorption to lower field and electron donating groups shift the absorption to higher field because of the local diamagnetic shielding effect. The position of absorption of an aromatic proton depends on at least three factors, the diamagnetic shielding, which is the most important and depends on the electron density at the carbon atom to which the proton is attached, paramagnetic shielding as a result of the ring current, whose magnitude will be greater for electron releasing substituent groups than for electron withdrawing substituent groups and a possible diamagnetic anisotropic effect, which will be greatest at position *ortho* to the substituent group. The presence of aromatic moieties in the curcumin molecule is confirmed by the absorption in the characteristic region. Aromatic nuclei contain large closed loop of

TABLE-2
VIBRATIONAL BAND ASSIGNMENT OF CURCUMIN

Frequency (cm ⁻¹)		Assignment
Calcd. (MM3)	Observed (FTIR)	
3555 m	3551 w	OH <i>str.</i>
3091 m	3183 w	Aromatic C-H <i>str.</i>
2962 m	2933 w	Aromatic C-H <i>str.</i>
2957 m	2923 w	Asymmetric CH <i>str.</i> of CH ₃ group
2872 w	2852 w	Symmetric CH <i>str.</i> of CH ₃ group
1712 m	1714 vw	Alkene C=C <i>str.</i> vibration
1675 vs	1626 s	C=O <i>str.</i>
1610 m	1602 s	C=O <i>str.</i>
1603 m	1583 s	C=O <i>str.</i>
1513 m	1509 vs	Aromatic C-C <i>str.</i>
1458 w	1460 m	Aromatic C-C <i>str.</i>
1446 w	1450 m	Aromatic C-C <i>str.</i>
1429 w	1429 s	In plane O-H deformation
1368 w	1373 w	Alkene CH ₂ scissoring
1314 w	1313 w	Alkene CH ₂ scissoring
1260 m	1275 s	C-O <i>str.</i>
1239 w	1233 m	C-O <i>str.</i>
1197 w	1206 m	Aromatic C-H in plane deformation
1171 m	1185 m	Aromatic C-H in plane deformation
1165 m	1167 m	Aromatic C-H in plane deformation
1154 m	1142 s	Aromatic C-H in plane deformation
1111 w	1113 m	Aromatic C-H out of plane deformation
1065 vw	1093 m	Aromatic C-H out of plane deformation
1036 m	1025 w	Aromatic C-H out of plane deformation
962 w	966 w	Alkene CH ₂ out of plane bending
957 w	961 w	Alkene CH ₂ out of plane bending
884 w	873 vw	CH inplane bending
846 w	855 vw	CH inplane bending
827 m	829 w	CH inplane bending
821 m	815 w	CH inplane bending
762 vw	786 w	CH out of plane bending
758 vw	753 vw	CH out of plane bending
735 w	725 vw	CH out of plane bending
675 w	660 vw	C-C in plane bending
642 w	640 vw	C-C-C in plane bending
613 w	620 vw	C-C-C in plane bending
597 w	606 vw	C-C-C in plane bending
564 w	572 vw	Aromatic C-C-C out of plane bending
556 w	564 vw	Aromatic C-C-C out of plane bending
540 w	541 vw	Aromatic C-C-C out of plane bending
511 w	512 vw	Aromatic C-C-C out of plane bending
507 w	506 vw	Aromatic C-C out of plane bending
481 w	475 w	Aromatic C-C out of plane bending
469 w	469 vw	Aromatic C-C out of plane bending

TABLE-3
CHEMICAL SHIFTS AND ASSIGNMENT OF PROTON SIGNALS
SHOWED IN ^1H NMR SPECTRUM OF CURCUMIN

Chemical shift δ (ppm)	Structural unit
a = 5.8	a b c b a
b = 1.8-3	H H O O H H
c = 1.26	-C=C-C-(CH ₂)-C-C=C
Aromatic protons 6.5-7.6	
d = 2.5-3.5	
e = 4	

π -electrons in which strong diamagnetic currents are induced by the magnetic field. This effect results in a paramagnetic shielding at the aromatic proton and is called the ring current effect. Hence any group that is sterically held above or below the plane of the aromatic nucleus will, obviously, be abnormally shielded because of the ring current effect. The presence of phenolic proton in curcumin is shown by the absorption in the ^1H MNR spectrum at 4 δ which is shifted to a higher field because of the local diamagnetic shielding effect.

Molecular mechanics

Computations were performed using computer program (MM3) of Allinger³³. In the methodology of computations, the total energy is calculated as a sum of terms corresponding to compression, bending, Van der Waal and dipole energies. Minimization of these terms relative to a strainless set by successive alteration in atomic coordinates leads to a configuration of minimum steric energy.

Optimized geometry: In the present investigation, the optimized geometrical parameters namely bond lengths and bond angles have been calculated for a particular conformation of the curcumin molecule using mole-cular mechanics method are presented in Table-4. The geometry and numbering of atoms of curcumin are presented in Fig. 1.

Thermodynamic properties: The total energy of a molecule is the sum of translational, rotational, vibrational and electronic energies, *i.e.*

$$E = E_t + E_r + E_v + E_e$$

Thus, the molecular partition function is the product of the translational, rotational, vibrational and electronic partition functions of the molecule. The relations between partition functions and various thermodynamic functions were used to evaluate the latter due to translation, vibration and rotation degrees of freedom of molecular motions. The statistical thermodynamic

TABLE-4
GEOMETRY PARAMETERS OF CURCUMIN

Bond type	Molecular parameter (Å)	Bond type	Molecular parameter (Å)	Bond type	Molecular parameter (Å)
C ₁ - C ₂	1.4064	O ₉ - H ₃₅	0.9717	C ₁₉ - C ₂₀	1.3952
C ₁ - C ₃	1.4038	C ₁₀ - C ₁₁	1.3455	C ₁₉ - C ₂₁	1.3951
C ₁ - C ₁₀	1.4790	C ₁₀ - H ₃₆	1.1039	C ₁₉ - H ₄₁	1.1031
C ₂ - C ₄	1.4015	C ₁₁ - C ₁₂	1.3616	C ₂₀ - C ₂₂	1.4018
C ₂ - H ₂₉	1.0996	C ₁₁ - H ₃₇	1.1006	C ₂₀ - O ₂₅	1.3623
C ₃ - C ₅	1.3935	C ₁₂ - C ₁₃	1.5272	C ₂₁ - C ₂₃	1.4044
C ₃ - H ₃₀	1.1033	C ₁₂ - O ₁₅	1.2166	C ₂₁ - H ₄₂	1.1032
C ₄ - C ₆	1.4016	C ₁₃ - C ₁₄	1.5278	C ₂₂ - C ₂₄	1.3976
C ₄ - O ₇	1.3680	C ₁₃ - H ₂₈	1.1141	C ₂₂ - O ₂₆	1.3647
C ₅ - C ₆	1.3983	C ₁₃ - H ₃₈	1.1095	C ₂₃ - C ₂₄	1.4061
C ₅ - H ₃₁	1.1033	C ₁₄ - C ₁₆	1.3616	C ₂₄ - H ₄₃	1.1013
C ₆ - O ₉	1.3629	C ₁₄ - O ₁₇	1.2164	O ₂₅ - H ₄₄	0.9741
O ₇ - C ₈	1.4169	C ₁₆ - C ₁₈	1.3450	O ₂₆ - C ₂₇	1.4188
C ₈ - H ₃₂	1.1136	C ₁₆ - H ₃₉	1.1007	C ₂₇ - H ₄₅	1.1144
C ₈ - H ₃₃	1.1131	C ₁₈ - C ₂₃	1.4809	C ₂₇ - H ₄₆	1.1134
C ₈ - H ₃₄	1.1097	C ₁₈ - H ₄₀	1.1039	C ₂₇ - H ₄₇	1.1097
Bond type	Bond angle (°)	Bond type	Bond angle (°)	Bond type	Bond angle (°)
C ₂ -C ₁ -C ₃	118.31	C ₁ -C ₁₀ -C ₁₁	124.85	C ₂₀ -C ₁₉ -H ₄₁	119.83
C ₂ -C ₁ -C ₁₀	122.68	C ₁ -C ₁₀ -H ₃₆	116.95	C ₂₁ -C ₁₉ -H ₄₁	119.81
C ₃ -C ₁ -C ₁₀	118.99	C ₁₁ -C ₁₀ -H ₃₆	118.17	C ₁₉ -C ₂₀ -C ₂₂	119.47
C ₁ -C ₂ -C ₄	121.22	C ₁₀ -C ₁₁ -C ₁₂	122.09	C ₁₉ -C ₂₀ -O ₂₅	118.68
C ₁ -C ₂ -H ₂₉	119.38	C ₁₀ -C ₁₁ -H ₃₇	120.81	C ₂₂ -C ₂₀ -O ₂₅	121.83
C ₄ -C ₂ -H ₂₉	119.38	C ₁₂ -C ₁₁ -H ₃₇	117.07	C ₁₉ -C ₂₁ -C ₂₃	120.88
C ₁ -C ₃ -C ₅	120.85	C ₁₁ -C ₁₂ -C ₁₃	116.78	C ₁₉ -C ₂₁ -H ₄₂	119.02
C ₁ -C ₃ -H ₃₀	120.04	C ₁₁ -C ₁₂ -O ₁₅	122.05	C ₂₃ -C ₂₁ -H ₄₂	120.06
C ₅ -C ₃ -H ₃₀	119.10	C ₁₃ -C ₁₂ -O ₁₅	121.15	C ₂₀ -C ₂₂ -C ₂₄	119.76
C ₂ -C ₄ -C ₆	119.43	C ₁₂ -C ₁₃ -C ₁₄	114.31	C ₂₀ -C ₂₂ -O ₂₆	120.23
C ₂ -C ₄ -O ₇	123.56	C ₁₂ -C ₁₃ -H ₂₈	109.07	C ₂₄ -C ₂₂ -O ₂₆	119.29
C ₆ -C ₄ -O ₇	116.99	C ₁₂ -C ₁₃ -H ₃₈	108.60	C ₁₈ -C ₂₃ -C ₂₁	119.06
C ₃ -C ₅ -C ₆	120.33	C ₁₄ -C ₁₃ -H ₂₈	109.26	C ₁₈ -C ₂₃ -C ₂₄	122.74
C ₃ -C ₅ -H ₃₁	119.23	C ₁₄ -C ₁₃ -H ₃₈	109.15	C ₂₁ -C ₂₃ -C ₂₄	118.19
C ₆ -C ₅ -H ₃₁	120.43	H ₂₈ -C ₁₃ -H ₃₈	106.10	C ₂₂ -C ₂₄ -C ₂₃	121.02
C ₄ -C ₆ -C ₅	119.82	C ₁₃ -C ₁₄ -C ₁₆	116.10	C ₂₂ -C ₂₄ -H ₄₃	118.19
C ₄ -C ₆ -O ₉	119.22	C ₁₃ -C ₁₄ -O ₁₇	121.99	C ₂₃ -C ₂₄ -H ₄₃	120.77
C ₅ -C ₆ -O ₉	120.95	C ₁₆ -C ₁₄ -O ₁₇	121.90	C ₂₀ -O ₂₅ -H ₄₄	109.02
C ₄ -O ₇ -C ₈	120.56	C ₁₄ -C ₁₆ -C ₁₈	122.03	C ₂₂ -O ₂₆ -C ₂₇	114.14
O ₇ -C ₈ -H ₃₂	110.82	C ₁₄ -C ₁₆ -H ₃₉	117.15	O ₂₆ -C ₂₇ -H ₄₅	110.70
O ₇ -C ₈ -H ₃₃	110.83	C ₁₈ -C ₁₆ -H ₃₉	120.80	O ₂₆ -C ₂₇ -H ₄₆	110.71
O ₇ -C ₈ -H ₃₄	109.03	C ₁₆ -C ₁₈ -C ₂₃	124.84	O ₂₆ -C ₂₇ -H ₄₇	109.31
H ₃₂ -C ₈ -H ₃₃	110.13	C ₁₆ -C ₁₈ -H ₄₀	118.23	H ₄₅ -C ₂₇ -H ₄₆	109.25
H ₃₂ -C ₈ -H ₃₄	107.96	C ₂₃ -C ₁₈ -H ₄₀	116.90	H ₄₅ -C ₂₇ -H ₄₇	108.41
H ₃₃ -C ₈ -H ₃₄	107.95	C ₂₀ -C ₁₉ -C ₂₁	120.34	H ₄₆ -C ₂₇ -H ₄₇	108.37
C ₆ -O ₉ -H ₃₅	112.53	—	—	—	—

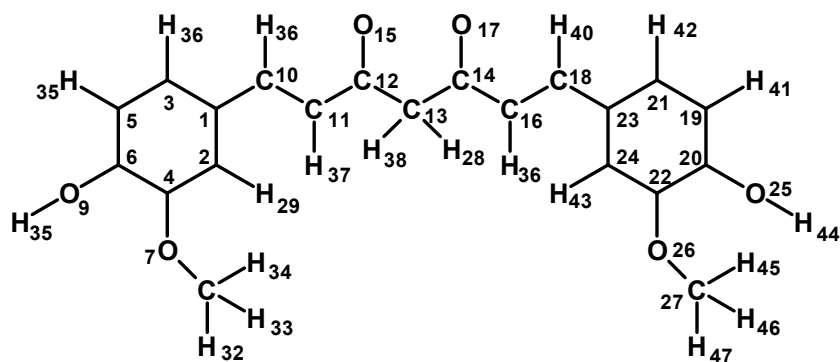


Fig. 1. Geometry and numbering of atoms of curcumin molecule

analysis of curcumin is carried out considering the molecule to be at room temperature of 298 K and one atmospheric pressure. In the methodology of MM3 computations, the contributions due to internal rotations are not considered. The free energy of the molecule is calculated including zero point energy and steric energy. The zero point energy of the molecule is 227.059 Kcal/mol. Molecular mechanics has been applied also to study the thermodynamic functions namely, enthalpy, entropy and heat capacity of the molecule curcumin and are presented in Table-5.

TABLE-5
THERMODYNAMIC FUNCTIONS OF CURCUMIN

Function	Energy (Kcal/mol)	Enthalpy (Kcal/mol)	Entropy (eu)	Free energy (Kcal/mol)	Heat capacity (cal/mol/deg)
Translational	0.889	1.481	43.583	-11.514	4.967
Rotational	0.889	0.889	37.144	-10.186	2.980
Vibrational	240.457 [†]	240.457 [†]	86.086	214.790 [†]	87.633
Potential	21.869 [‡]	21.869 [‡]	0.000	21.869 [‡]	0.000
Mixing	0.000	0.000	1.377	-0.411	0.000
Total	264.104	264.696	168.190	214.549	95.581

[†]Includes zero point energy (ZPE); [‡]Includes steric energy (SE), Internal rotation contributions are not considered).

Steric energy analysis: The total steric energy for the optimized geometry of the molecule is the most widely used data from MM3 calculations. MM3 force field includes terms for vibrational bond stretching, bond angle bending, torsional vibration, interactions between atoms of a molecule that are not bonded to each other, stretching bending vibrations, bend-bend and torsional-stretch to describe the potential energy of the molecule in various

conformations and this helps in identifying specific sites and types of strain. The steric energy is calculated for the curcumin molecule and the results are presented in Table-6. The steric energy of initial conformation of curcumin was 189.3556 kcal. Geometry minimization is done using full matrix optimizer till the lowest steric energy is reached. The final steric energy was 21.8689 kcal which is a local minimum, *i.e.*, geometry with energy lower than that of any similar geometry for curcumin. The minimum steric energy of a molecule gives the most stable configuration of the molecule structure.

TABLE-6
STERIC ENERGY OF CURCUMIN

Components of steric energy	MM3 Calculated values (kcal)
Compression	1.5048
Bending	5.5425
Bend-Bend	-0.0005
Stretch-Bend	-0.0330
Vanderwaals 1,4 Energy	20.6978
Other	1.8936
Torsional	-12.4891
Torsion-Stretch	-0.0067
Dipole-Dipole	4.7594
Charge-Dipole	0.0000
Charge-Charge	0.0000

Moment of inertia and dipole moment: The values of moment of inertia along the three principal axes, I_x , I_y and I_z have been calculated and are found to be 222.2251, 1706.2470 and 1797.7140 g/cm², respectively. Since, $I_x < I_y < I_z$ the molecule may be classified as spherical top. The dipole moment of the molecule is found to be 4.5627 D.

The present investigation deals with the characterization of the curcumin by UV-Visible, FTIR and FT-NMR spectroscopic methods. A complete vibrational band assignment has been made available for curcumin using FTIR spectral data. The experimental IR data has been well supported by the theoretical frequencies obtained by molecular mechanics calculations. The expected enol configuration of curcumin, in analogy with the other β -diketones is confirmed by the NMR spectral data.

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