

Theoretical Calculations of Vibration Modes and Electronic Properties of (1G) Dendrimers

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Abstract: *Semi-empirical method (PM3) was realized to estimate the (3N-6) frequencies of vibration modes and intensities of absorption in Infra-Red (IR) at equilibrium geometries, of unique architectural design of poly methyl methacrylate (1G) dendrimers (PMMA) molecule high degree of branching, multivalency. The Gaussian03 and MOPAC appraisement Packages have been performed throughout this analysis to estimate the Parameters geometrically (bond angle and bond lengths) and the physical properties, (vibration frequency, heat of formation and electronic charge distribution for the Dendrimer (PMMA) ($C_{15}H_{33}N_7O_3$) molecule. All the irreducible representations of vibration modes were assigned according to the group theory and character tables. Electronic Charge density at the atoms have also been calculated and presented graphically. The importance of this nano size molecule based on the extensive applications in various technological and industrial fields, is ascribed to the novel mechanical, electronic, physical, thermal properties, optical materials, laser applications and in medical treatment like drug surrender, tumor therapy, gene movement, Medical diagnostics and chemical catalysis.*

Keywords: (PMMA) Dendrimer, Gaussian03 program, Nanoparticle, MOPAC program

1. Introduction

The chemistry of dendrimers chemistry Science started by Fritz Vogtle and co-workers in 1978 [1], the first family of dendrimers feigned in 1985 by Donald A. Tomalia, [2]. The word dendrimer which means to "tree" comes from a Greek word. Dendrimer the synthetic polymer is a greatly branched and compos of unit of monomer bounded core, where a conductive to a mono model, like tree, shap as star or interpolation system with molecular weights accurately, diameters with range sizes between 2 to 10 nm, its singular architectonic scheme, branching with great degree, diverse valency, globular system of a modern section of science of polymer [3]. General dendrimers (PMMA) molecules are polymers of the esters of methacrylic acids. The greatest commonly used midst them is poly (methyl methacrylate) (PMMA) with chemical formula $C_{15}H_{33}N_7O_3$. The growth of functional nanoparticles is of more important benefit because it was discovered that the distinctive properties of such nanoscale substance to enable advance in Nanotechnology, life sciences and bioengineering. To tune the properties of the nano-particles for particular applications, not only the chemical construction of molecule but also the nano-size of the systems to require to be well examined. Structural approaches guide to a branched structure by unique a special characteristic responsibil change the form, polarity, size, shape properties and inner structure. These a special characteristic of (PMMA) make it applicable for long open-air action of operating. Nanoparticle drug-surrender systems are the of the general public ones able to raise the selection and fixity of therapeutic instrument. Dendrimer (PMMA) is one of polymers that is the greatest counteractive to direct sunshine incurrence. Its strength features demonstrate with justice little difference under the impact of UV-radiation, in addition to being there of ozone[4]. The drug- salutation systems with Nanoparticles are of great extent appreciated ones are capable growth selective and durability of curative agents. The agents with bioactive can be encapsulated the dendrimers in the interior. Conjugated and physical therapy adsorbed onto surface of dendrimer, tending required a

special characteristic of gravidbearer to particular requirement forceful substance and its curative. Controlling intermolecular interactions is one of the key issues for applying optical materials based on isolated electron system (eg. organic molecules and quantum dots) to photonic devices. Dendrimers of adequate molecular weight have e on a spherical shape because of dilation of the molecular chains [5-8]. Constructed by branched technique, beginning from starter core chemical agents as if ammonia. When viewing at construction in two-dimensions of a high generation, observed like star model (Fig.1). They are mercantile obtained in generation G0- G10 with G5 variant core kind and 10 functional groups level [9, 10], possess fast and competent optical functions founding from the resonance of separated electrons in π -conjugated systems. These characteristics make these materials strong candidates for use in optical control devices for ultrahigh-speed communications. However, orbitals of the π electrons, being subject to the molecular face, are handily affected by surrounding media, origin, adjacent molecules, and other element, which may have an effect in changes in optical responses. For this cause, command of intermolecular interactions forces is an important subject in the incorporation of extremely functional molecules into apparatus. Interaction command in nanoscale gap has also drawn attention in inorganic materials, including functional applications of separated electron systems like quantum dots[11]. Dendrimer is in analogous about core (fig1), frequently define with three dimensional. The point of view chemistry of polymer dendrimeres were absolute mono scatter huge molecules usual with great forked three dimensional construction (figure2) it comprise three construction segments like core, embranchment, final groups [12,13]. Dendrimers which have not high generations (G0, G1, and G2) have extremely asymmetric structure have greater accessible structures like collated of great generation dendrimers. The bobstay increasing from the core come to be of great length and higher branchy (in G4 with higher generations) dendrimers comply globular shape [14]. Dendrimers come to be overcrowded with densely when it expand in outer area, this shape like a closed - layer as

structure. When of criticism branchy case is arrived dendrimers cannot increase due to poverty of gap [14].

2. Methods of Calculation

All calculations were performed using a program of Pople et al. named Gaussian03. [15], and the program of P. Bischof, Heidelberg (Molek 9000), using these Computational collection have been employed during this study to compute the geometric data (bond lengths and angles) the electronic properties and Mulliken atomic charges were practical during the present study[16].

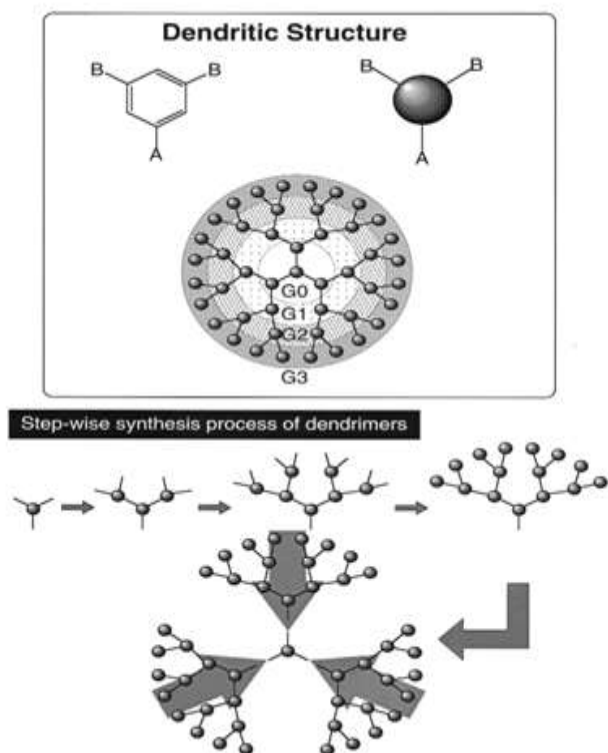


Figure 1: Structure of a dendrimer (PMMA)

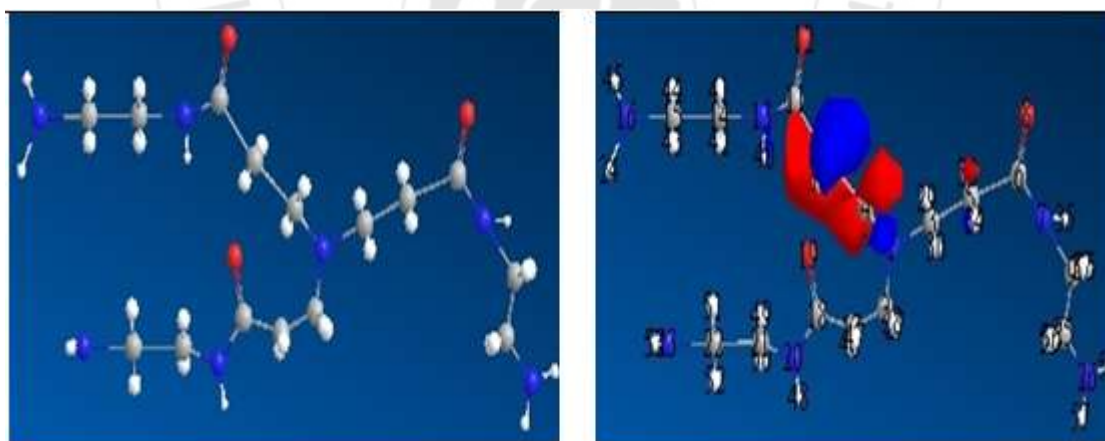


Figure 2: Equilibrium geometry for dendrimer (G1) (PMMA) applying G03 program

3. Results and Discussion

The first-generation dendrimer (G1), used in this study of present work we analysis the vibration frequencies values of dendrimer (G1), one be forced determine its geometric data first , study the correlation among vibration motion modes and the electronic properties. Interactions of (PMMA) C=O groups and dendrimer N-H groups contributed to miscibility. Obviously, the vibration of Dendrimers (PMMA) reasons a deformation in its geometry to transfer their electronic and thermal properties [17].

Table 1: show the main physical properties of Poly(methyl methacrylate) molecule which calculated in our study, E=energy of (PMMA) H= heat of formation ,G= gipes energy, S= entropy. The value of these parameters revealed Dendrimers (PMMA) has high mechanical strength and electrical properties. The point group of the molecule is C1.

Table 1: Physical properties of dendrimer G1 (PMMA) calculated by G03 program.

E (kJ/mol)	H (KJ/mol)	G (KJ/mol)	C _V (J/mol.K)	C _P (J/mol.K)	S (J/mol.K)
1366.582	1369.061	1134.161	430.151	438.465	787.858

Table 2: Calculated thermol parameters of dendrimer (G1) (PMMA) by G03 program

Total Energy	Heat Capacity	Molecular Mass	Thermodynamic Energy	Dipole/Dipole
1991.496 kcal/mol	90.336 Cal/mol-Kelvin	359.264 amu.	354.095 Kcal/mol	- 5.148a.u.

Dendrimers reveal some important improved chemical and physical characteristic when compared to classical linear polymers. Table 3. Show the calculated bond length and Bond angles show that C-C bond length is the highest bond in Dendrimers (PMMA) molecule, then C-N bond length, finally C-H bond length. Furthermore, symmetry in bond length and angels in the Dendrimers (PMMA) molecule caused unusual physical properties for Dendrimers (PMMA) molecule.

Table 3: Calculated geometry for dendrimers (PMMA) molecule by G03 program

Bond length (A°) and Bond angles (deg.)	bond length
N1-C2	1.438
N1-C3	1.438
N1-C4	1.438
N1-Lp59	0.600
C2-C17	1.523
C2-H26	1.113
C2-H27	1.113
C3-C5	1.523
C3-H28	1.113
C3-H29	1.113
C4-C10	1.523
C4-H30	1.113
C4-H31	1.113
C5-C6	1.509
C5-H32	1.113
C5-H33	1.113
C6-N7	1.369
C6-O8	1.208
N7-C9	1.460
N7-H34	1.022
C9-C24	1.523
C9-H35	1.113
C9-H36	1.113
C10-C11	1.509
C10-H37	1.113
C10-H38	1.113
C11-O12	1.208
C11-N13	1.369
N13-C14	1.460
N13-H39	1.022
C14-C15	1.523
C14-H40	1.113
C14-H41	1.113
C15-N16	1.468
C15-H42	1.113
C15-H43	1.113
N16-H44	1.035
N16-H45	1.035
N16-Lp60	0.600
C17-C18	1.509
C17-H46	1.113
C17-H47	1.113
C18-O19	1.208
C18-N20	1.369

N ₂₀ -C ₂₁	1.460
N ₂₀ -H ₄₈	1.022
C ₂₁ -C ₂₂	1.523
C ₂₁ -H ₄₉	1.113
C ₂₁ -H ₅₀	1.113
C ₂₂ -N ₂₃	1.468
C ₂₂ -H ₅₁	1.113
C ₂₂ -H ₅₂	1.113
N ₂₃ -H ₅₃	1.035
N ₂₃ -H ₅₄	1.035
N ₂₃ -Lp ₆₁	0.600
C ₂₄ -N ₂₅	1.468
C ₂₄ -H ₅₅	1.113
C ₂₄ -H ₅₆	1.113
N ₂₅ -H ₅₇	1.035
N ₂₅ -H ₅₈	1.035
N ₂₅ -Lp ₆₂	0.600
bond angle	
C ₂ -N ₁ -C ₃	107.700°
C ₂ -N ₁ -C ₄	107.700°
C ₂ -N ₁ -Lp ₅₉	109.200
C ₃ -N ₁ -C ₄	107.700°
C ₃ -N ₁ -Lp ₅₉	109.200°
C ₄ -N ₁ -Lp ₅₉	109.200°
N ₁ -C ₂ -C ₁₇	109.500°
C ₁₇ -C ₂ -H ₂₆	109.410°
C ₁₇ -C ₂ -H ₂₇	109.410°
H ₂₆ -C ₂ -H ₂₇	109.400°
N ₁ -C ₃ -C ₅	109.500°
C ₅ -C ₃ -H ₂₈	109.410°
C ₅ -C ₃ -H ₂₉	109.410°
H ₂₈ -C ₃ -H ₂₉	109.400°
N ₁ -C ₄ -C ₁₀	109.500°
C ₁₀ -C ₄ -H ₃₀	109.410°
C ₁₀ -C ₄ -H ₃₁	109.410°
H ₃₀ -C ₄ -H ₃₁	109.400°
C ₃ -C ₅ -C ₆	110.000°
C ₃ -C ₅ -H ₃₂	109.410°
C ₃ -C ₅ -H ₃₃	109.410°
C ₆ -C ₅ -H ₃₂	108.800°
C ₆ -C ₅ -H ₃₃	108.800°
H ₃₂ -C ₅ -H ₃₃	109.400°
C ₅ -C ₆ -N ₇	114.000°
C ₅ -C ₆ -O ₈	122.500°
N ₇ -C ₆ -O ₈	122.600°
C ₆ -N ₇ -H ₃₄	117.400°
C ₉ -N ₇ -H ₃₄	118.000°
N ₇ -C ₉ -C ₂₄	109.280°
C ₂₄ -C ₉ -H ₃₅	109.410°
C ₂₄ -C ₉ -H ₃₆	109.410°
H ₃₅ -C ₉ -H ₃₆	109.400°
C ₄ -C ₁₀ -C ₁₁	110.000°
C ₄ -C ₁₀ -H ₃₇	109.410°
C ₄ -C ₁₀ -H ₃₈	109.410°
C ₁₁ -C ₁₀ -H ₃₇	108.800°
C ₁₁ -C ₁₀ -H ₃₈	108.800°
H ₃₇ -C ₁₀ -H ₃₈	109.400°
C ₁₀ -C ₁₁ -O ₁₂	122.500°
C ₁₀ -C ₁₁ -N ₁₃	114.000°
O ₁₂ -C ₁₁ -N ₁₃	122.600°

information of valence shape of each vibration motion to enable a connected comparison of modes and accordingly the force constants and bond strengths within molecule[22]. The effected vibrational motion modes in the (PMMA) were C-H symmetric stretching which corresponds to C=O stretching band and correspond to C—O stretching modes (fig.4). The vibrations caused by deformation modes of CH₃ groups [23].

Show the calculated Atomic electronic density and charge on (PMMA) atoms by G03 program. Finally, the calculations show that, the calculated charge and Atomic electronic density in (PMMA) atoms employing G03 program[24]. The charge densities are chiefly collected in the O atom, then N atom and finally on C atom (table 5). From the calculated Mulliken atomic charges for (PMMA) it is found that H atoms have positive charge and other atoms have negative charge that fact lead to (PMMA) is especially known for its exceptional optical properties. (table 5).

Fig.4 shows some vibration modes for Dendrimers (PMMA) molecule as calculated applying G03 program.. Table 5.

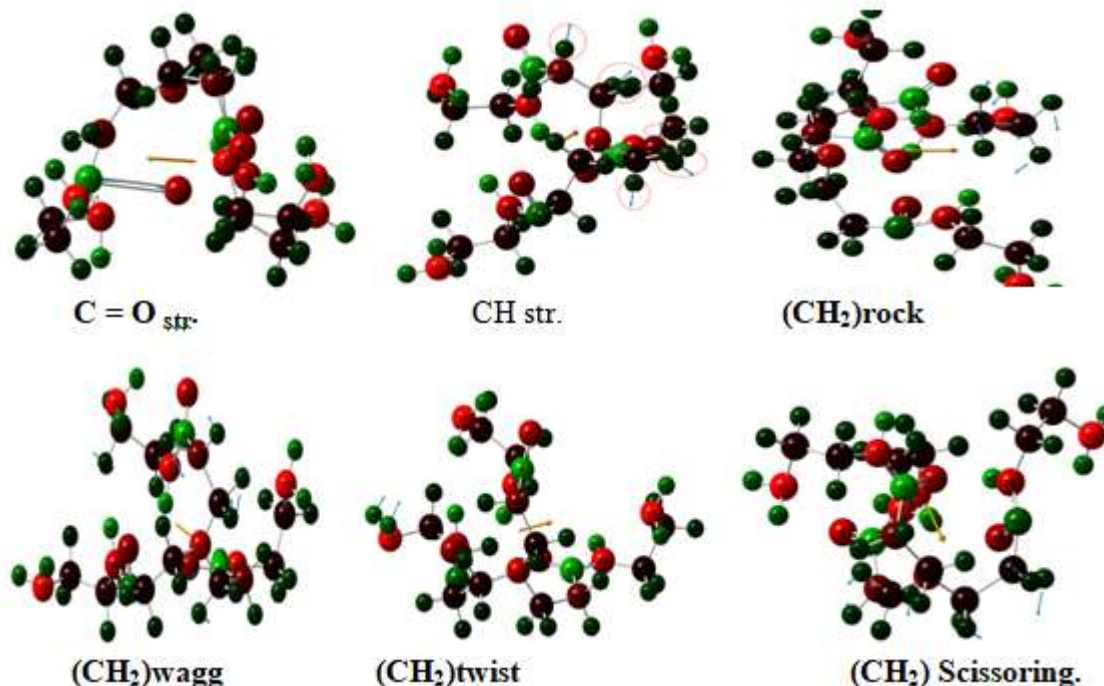


Figure 4: The graphical pictures of some vibration modes for Dendrimers (PMMA) calculated applying G03 program

Table 4: The Vibrational frequencies and IR absorption intensities values for Dendrimers G1(PMMA) calculated applying G03program.

<i>Symmetry and description</i>	<i>Frequency cm⁻¹</i>	<i>Intensity km/mol</i>
v ₁	ρ(CH ₂)rock	11.642
v ₂	ρ(CH ₂)rock	16.556
v ₃	ρ(CH ₂)rock	17.904
v ₄	ρ(CH ₂)rock	26.567
v ₅	ρ(CH ₂)rock	30.752
v ₆	ρ(CH ₂)rock	39.834
v ₇	γ NH	50.063
v ₈	γ NH	55.241
v ₉	γ NH	61.382
v ₁₀	γ NH	71.745
v ₁₁	γ NH	87.196
v ₁₂	γ NH	98.102
v ₁₃	δ(CH)	106.924
v ₁₄	ρ(CH ₂) rock	118.263
v ₁₅	ρ(CH ₂) rock	120.493
v ₁₆	ρ(CH ₂) rock	131.048
v ₁₇	ρ(CH ₂) rock	161.344
v ₁₈	ρ(CH ₂) rock	173.341
v ₁₉	ρ(CH ₂) rock	184.212
v ₂₀	ρ(CH ₂) rock	193.175
v ₂₁	ρ(CH ₂) rock	206.737
v ₂₂	ρ(CH ₂) rock	219.145

v ₂₃	ρ(CH ₂) rock	229.048	6.267
v ₂₄	ρ(CH ₂) rock	249.654	8.218
v ₂₅	ρ(CH ₂) rock	263.727	2.955
v ₂₆	ρ(CH ₂) rock	271.742	35.447
v ₂₇	ρ(CH ₂) rock	291.743	13.247
v ₂₈	ρ(CH ₂) rock	296.291	2.259
v ₂₉	ρ(CH ₂) rock	316.406	1.811
v ₃₀	ρ(CH ₂) rock	328.122	68.865
v ₃₁	ρ(CH ₂) rock	337.764	4.398
v ₃₂	ρ(CH ₂) rock	357.034	2.483
v ₃₃	ρ(CH ₂) rock	392.502	2.318
v ₃₄	ρ(CH ₂) rock	406.355	16.017
v ₃₅	ρ(CH ₂) rock	413.256	3.099
v ₃₆	ρ(CH ₂) rock	460.790	1.723
v ₃₇	τ(CH ₂) twist.	489.287	24.112
v ₃₈	ρ(CH ₂) rock	495.483	39.570
v ₃₉	ρ(CH ₂) rock	529.209	3.365
v ₄₀	ρ(CH ₂) rock	530.947	1.406
v ₄₁	ρ(CH ₂) rock	560.760	27.551
v ₄₂	ρ(CH ₂) rock	571.037	10.491
v ₄₃	ρ(CH ₂) rock	595.289	6.840
v ₄₄	ω(CH ₂).wagging	608.167	33.969
v ₄₅	ω(CH ₂).wagging	610.457	185.400
v ₄₆	ω(CH ₂).wagging	640.587	134.341
v ₄₇	ω(CH ₂).wagging	658.462	15.376
v ₄₈	ω(CH ₂).wagging	689.015	7.247
v ₄₉	ω(CH ₂).wagging	709.448	370.185

V ₅₀	$\tau(\text{CH}_2)\text{twist.}$	746.686	21.713
V ₅₁	$\rho(\text{CH}_2)\text{rock.}$	765.661	173.990
V ₅₂	$\rho(\text{CH}_2)\text{rock.}$	786.476	168.311
V ₅₃	$\tau(\text{CH}_2)\text{twist.}$	808.642	25.282
V ₅₄	$\tau(\text{CH}_2)\text{twist.}$	855.063	75.859
V ₅₅	$\tau(\text{CH}_2)\text{twist.}$	871.786	72.725
V ₅₆	$\tau(\text{CH}_2)\text{twist.}$	886.543	8.061
V ₅₇	$\tau(\text{CH}_2)\text{twist.}$	889.161	0.723
V ₅₈	$\tau(\text{CH}_2)\text{twist.}$	930.465	14.750
V ₅₉	$\tau(\text{CH}_2)\text{twist.}$	936.438	8.885
V ₆₀	$\tau(\text{CH}_2)\text{twist.}$	951.827	87.485
V ₆₁	$\rho(\text{CH}_2)\text{rock.}$	974.548	101.131
V ₆₂	$\tau(\text{CH}_2)\text{twist.}$	987.600	2.442
V ₆₃	$\rho(\text{CH}_2)\text{rock.}$	1004.496	30.824
V ₆₄	$\tau(\text{CH}_2)\text{twist.}$	1006.189	3.502
V ₆₅	$\rho(\text{CH}_2)\text{rock.}$	1031.610	3.357
V ₆₆	$\rho(\text{CH}_2)\text{rock.}$	1053.167	7.873
V ₆₇	$\rho(\text{CH}_2)\text{rock.}$	1071.139	3.527
V ₆₈	$\tau(\text{CH}_2)\text{twist.}$	1074.475	9.158
V ₆₉	$\tau(\text{CH}_2)\text{twist.}$	1090.646	18.629
V ₇₀	$\rho(\text{CH}_2)\text{rock.}$	1117.454	13.486
V ₇₁	$\tau(\text{CH}_2)\text{twist.}$	1124.143	24.404
V ₇₂	$\tau(\text{CH}_2)\text{twist.}$	1152.310	64.709
V ₇₃	$\tau(\text{CH}_2)\text{twist.}$	1157.813	34.449
V ₇₄	$\tau(\text{CH}_2)\text{twist.}$	1162.972	71.317
V ₇₅	$\tau(\text{CH}_2)\text{twist.}$	1190.700	35.262
V ₇₆	$\tau(\text{CH}_2)\text{twist.}$	1195.607	9.062
V ₇₇	$\omega(\text{CH}_2)\text{wagg.}$	1200.976	36.855
V ₇₈	$\omega(\text{CH}_2)\text{wagg.}$	1214.970	44.133
V ₇₉	$\omega(\text{CH}_2)\text{wagg.}$	1217.243	111.358
V ₈₀	$\omega(\text{CH}_2)\text{wagg.}$	1224.316	245.251
V ₈₁	$\omega(\text{CH}_2)\text{wagg.}$	1234.615	7.147
V ₈₂	$\omega(\text{CH}_2)\text{wagg.}$	1239.484	10.722
V ₈₃	$\tau(\text{CH}_2)\text{twist.}$	1266.367	72.500
V ₈₄	$\tau(\text{CH}_2)\text{twist.}$	1273.535	15.538
V ₈₅	$\tau(\text{CH}_2)\text{twist.}$	1283.974	58.970
V ₈₆	$\tau(\text{CH}_2)\text{twist.}$	1300.802	1.779
V ₈₇	$\tau(\text{CH}_2)\text{twist.}$	1314.509	16.547
V ₈₈	$\tau(\text{CH}_2)\text{twist.}$	1321.052	1.172
V ₈₉	$\tau(\text{CH}_2)\text{twist.}$	1374.669	25.868
V ₉₀	$\tau(\text{CH}_2)\text{twist.}$	1383.675	9.508
V ₉₁	$\tau(\text{CH}_2)\text{twist.}$	1404.073	57.251
V ₉₂	$\tau(\text{CH}_2)\text{twist.}$	1411.474	53.863
V ₉₃	$\tau(\text{CH}_2)\text{twist.}$	1420.327	80.967
V ₉₄	$\tau(\text{CH}_2)\text{twist.}$	1421.429	30.532
V ₉₅	$\tau(\text{CH}_2)\text{twist.}$	1430.587	6.579
V ₉₆	$\tau(\text{CH}_2)\text{twist.}$	1447.869	35.390
V ₉₇	$\tau(\text{CH}_2)\text{twist.}$	1458.435	28.319
V ₉₈	$\tau(\text{CH}_2)\text{twist.}$	1459.407	16.854
V ₉₉	$\tau(\text{CH}_2)\text{twist.}$	1469.288	140.797
V ₁₀₀	$\omega(\text{CH}_2)\text{wagg.}$	1475.473	1.740
V ₁₀₁	$\omega(\text{CH}_2)\text{wagg.}$	1482.120	9.168
V ₁₀₂	$\tau(\text{CH}_2)\text{twist.}$	1499.712	39.672
V ₁₀₃	$\omega(\text{CH}_2)\text{wagg.}$	1500.388	37.110
V ₁₀₄	$\omega(\text{CH}_2)\text{wagg.}$	1506.099	29.328
V ₁₀₅	$\omega(\text{CH}_2)\text{wagg.}$	1523.698	6.370
V ₁₀₆	$\omega(\text{CH}_2)\text{wagg.}$	1544.017	33.274
V ₁₀₇	$\omega(\text{CH}_2)\text{wagg.}$	1547.495	4.304
V ₁₀₈	$\omega(\text{CH}_2)\text{wagg.}$	1550.786	19.277
V ₁₀₉	$\omega(\text{CH}_2)\text{wagg.}$	1555.056	2.852
V ₁₁₀	$\omega(\text{CH}_2)\text{wagg.}$	1563.202	4.510
V ₁₁₁	$\omega(\text{CH}_2)\text{wagg.}$	1564.267	17.673
V ₁₁₂	$\omega(\text{CH}_2)\text{wagg.}$	1570.310	12.878

V ₁₁₃	$\omega(\text{CH}_2)\text{wagg.}$	1571.941	16.274
V ₁₁₄	$\omega(\text{CH}_2)\text{wagg.}$	1585.022	152.323
V ₁₁₅	$\omega(\text{CH}_2)\text{wagg.}$	1590.189	2.916
V ₁₁₆	$\omega(\text{CH}_2)\text{wagg.}$	1621.770	7.232
V ₁₁₇	$\omega(\text{CH}_2)\text{wagg.}$	1633.13	30.323
		74	
V ₁₁₈	$\omega(\text{CH}_2)\text{wagg.}$	1637.849	7.472
V ₁₁₉	$\zeta(\text{CH}_2)\text{ Scissoring.}$	1641.624	2.380
V ₁₂₀	$\zeta(\text{CH}_2)\text{ Scissoring.}$	1645.390	4.803
V ₁₂₁	$\zeta(\text{CH}_2)\text{ Scissoring.}$	1656.773	7.359
V ₁₂₂	$\zeta(\text{CH}_2)\text{ Scissoring.}$	1662.916	12.709
V ₁₂₃	$\zeta(\text{CH}_2)\text{ Scissoring.}$	1665.468	10.563
V ₁₂₄	$\zeta(\text{CH}_2)\text{ Scissoring.}$	1668.976	3.084
V ₁₂₅	$\zeta(\text{CH}_2)\text{ Scissoring.}$	1670.219	8.130
V ₁₂₆	$\zeta(\text{CH}_2)\text{ Scissoring.}$	1675.335	6.447
V ₁₂₇	$\zeta(\text{CH}_2)\text{ Scissoring.}$	1676.179	5.647
V ₁₂₈	$\zeta(\text{CH}_2)\text{ Scissoring.}$	1689.909	4.221
V ₁₂₉	$\zeta(\text{CH}_2)\text{ Scissoring.}$	1708.164	278.366
V ₁₃₀	$\zeta(\text{CH}_2)\text{ Scissoring.}$	1730.951	305.540
V ₁₃₁	$\zeta(\text{CH}_2)\text{ Scissoring.}$	1833.449	307.972
V ₁₃₂	$\zeta(\text{NH}_2)\text{ Scissoring.}$	1842.598	369.351
V ₁₃₃	$\zeta(\text{NH}_2)\text{ Scissoring.}$	1846.376	48.229
V ₁₃₄	$\zeta(\text{NH}_2)\text{ Scissoring.}$	1847.151	105.238
V ₁₃₅	$\zeta(\text{NH}_2)\text{ Scissoring.}$	1864.745	38.903
V ₁₃₆	(O=C--N)str.	2138.660	135.966
V ₁₃₇	(O=C--N)str.	2146.810	101.233
V ₁₃₈	(O=C--N)str.	2167.040	38.657
V ₁₃₉	CH str.	3147.209	91.367
V ₁₄₀	CH str.	3156.575	49.615
V ₁₄₁	CH str.	3178.317	22.323
V ₁₄₂	CH str.	3185.021	71.395
V ₁₄₃	CH str.	3195.921	41.015
V ₁₄₄	CH str.	3202.411	23.342
V ₁₄₅	CH str.	3213.789	27.601
V ₁₄₆	CH str.	3214.915	28.417
V ₁₄₇	CH str.	3236.002	65.1639
V ₁₄₈	CH str.	3236.156	40.690
V ₁₄₉	CH str.	3251.477	38.258
V ₁₅₀	CH str.	3251.8646	32.477
V ₁₅₁	CH str.	3263.689	1.9762
V ₁₅₂	CH str.	3265.220	62.006
V ₁₅₃	CH str.	3268.588	12.801
V ₁₅₄	CH str.	3285.967	18.927
V ₁₅₅	CH str.	3287.368	19.339
V ₁₅₆	CH str.	3290.557	18.025
V ₁₅₇	CH str.	3311.726	5.852
V ₁₅₈	CH str.	3312.830	10.441
V ₁₅₉	CH str.	3334.031	23.451
V ₁₆₀	CH str.	3778.925	23.910
V ₁₆₁	CH str.	3784.673	41.577
V ₁₆₂	CH str.	3794.293	3.432
V ₁₆₃	CH str.	3812.932	5.290
V ₁₆₄	CH str.	3827.793	158.537
V ₁₆₅	CH str.	3851.030	36.092
V ₁₆₆	CH str.	3905.931	42.072
V ₁₆₇	CH str.	3913.241	10.522
V ₁₆₈	CH str.	3935.579	14.112

Table 5: Calculated charge and Atomic electron density on (PMMA) atoms using G03 program

Atom No. type	Charge	Mulliken atomic charges	Atomic electron density
N ₁	N 0.417	-0.265	5.090
C ₂	C -0.113	-0.047	4.087
C ₃	C 0.040	-0.047	4.067
C ₄	C 0.056	-0.043	4.066
C ₅	C 0.037	-0.153	4.130
C ₆	C -0.141	0.227	3.760
N ₇	N 0.006	-0.334	5.057
O ₈	O 0.026	-0.273	6.372
C ₉	C 0.005	-0.056	4.068
C ₁₀	C 0.015	-0.151	4.130
C ₁₁	C 0.195	0.240	3.759
O ₁₂	O -0.797	-0.258	6.375
N ₁₃	N 0.021	-0.317	5.061
C ₁₄	C 0.099	-0.042	4.062
C ₁₅	C 0.169	-0.053	4.113
N ₁₆	N 0.032	-0.397	5.025
C ₁₇	C 0.011	-0.034	4.125
C ₁₈	C 0.052	0.141	3.762
O ₁₉	O 0.014	-0.219	6.381
N ₂₀	N 0.026	-0.282	5.055
C ₂₁	C 0.380	-0.060	4.071
C ₂₂	C -0.832	-0.058	4.110
N ₂₃	N 0.013	-0.400	5.033
H ₂₄	H 0.095	0.162	4.109
C ₂₅	C 0.044	-0.056	5.029
N ₂₆	N 0.031	-0.407	0.940
H ₂₇	H 0.031	0.050	0.924
H ₂₈	H -0.289	0.073	0.919
H ₂₉	H 0.004	0.084	0.949
H ₃₀	H 0.027	0.056	0.949
H ₃₁	H 0.162	0.057	0.918
H ₃₂	H 0.023	0.085	0.932
H ₃₃	H 0.025	0.074	0.918
H ₃₄	H -0.642	0.082	0.924
H ₃₅	H 0.015	0.230	0.923
H ₃₆	H 0.017	0.084	0.938
H ₃₇	H 0.451	0.081	0.937
H ₃₈	H 0.189	0.078	0.921
H ₃₉	H 0.030	0.077	0.920
H ₄₀	H 0.097	0.206	0.941
H ₄₁	H 0.046	0.080	0.922
H ₄₂	H 0.032	0.089	0.972
H ₄₃	H 0.039	0.056	0.937
H ₄₄	H 0.283	0.079	0.974
H ₄₅	H 0.026	0.154	0.973
H ₄₆	H 0.028	0.045	0.920
H ₄₇	H 0.039	0.089	0.927
H ₄₈	H 0.028	0.219	0.920
H ₄₉	H 0.029	0.084	0.953
H ₅₀	H 0.288	0.064	0.916
H ₅₁	H 0.025	0.046	0.961
H ₅₂	H 0.005	0.074	0.945
H ₅₃	H 0.113	0.157	0.973
H ₅₄	H 0.112	0.155	0.970
H ₅₅	H 0.112	0.058	0.966
H ₅₆	H 0.112	0.077	0.947
H ₅₇	H 0.112	0.175	0.973
H ₅₈	H 0.112	0.155	0.972

5. Conclusions

Dendrimers (PMMA) is an economic, multiplex general purpose substance. It is available in cast material in layer, tube and rod shape, in addition to custom profiles. Different kinds of acrylics are adopted in a wide variety of fields and performances, containing: PMMA has high mechanical strength, The covers of a Lamp, parts of switch, dials, buttons which control and Optics: sunglasses for dust covers, lenses, watch glasses, adducting and glasses. The complete analysis of all vibration frequencies and normal coordinates of Dendrimers (PMMA.) yielded good frequency values using Gaussian 03 Program, The alteration in vibration frequencies modes of (N-C=O)str. bond is due to the change in the charge, bond order, force constant and bond lengths of the Dendrimers (PMMA). Fundamental vibrations of Dendrimers (PMMA) were calculated and specification like rocking, scissoring modes, twisting modes in C-H bonds, wagging modes in C-H bonds, γ NH, (O=C-N)str and CHstr. The calculations show that, calculated charge and Atomic electron density on Dendrimers (PMMA) atoms using G03 program. Considerably the charge densities are collected in O atom, then N atom and finally on C atom. The calculated Mullikan atomic charges for (PMMA) it is found that H atoms have positive charge and other atoms were have a negative charge that fact leads to exhibits very good optical and electrical properties.

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