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

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Abstract: ***Semi-empirical methode (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, electronicl, 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 C15H33N7O3. 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].

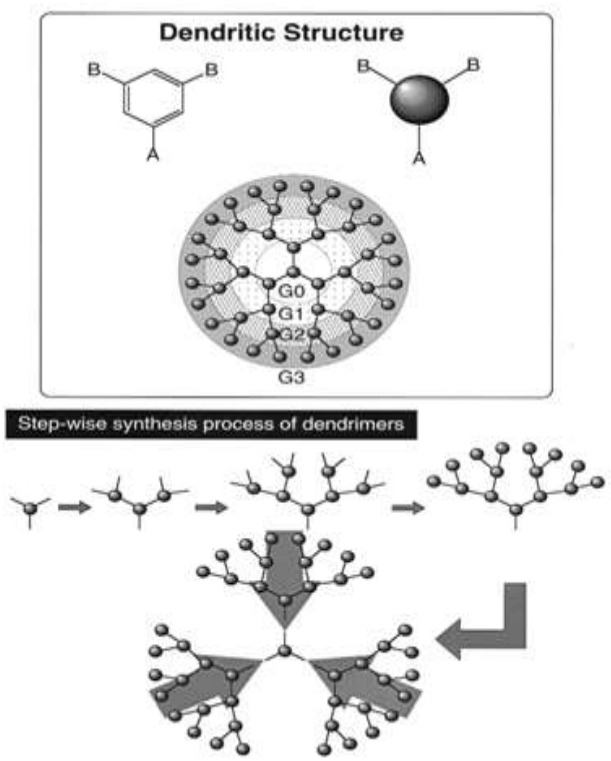

Figure 1: Structure of a dendrimer (PMMA)

2. Methods of Calculation

All calculations were performed using a program of Pople et al. named Guassian03. [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].

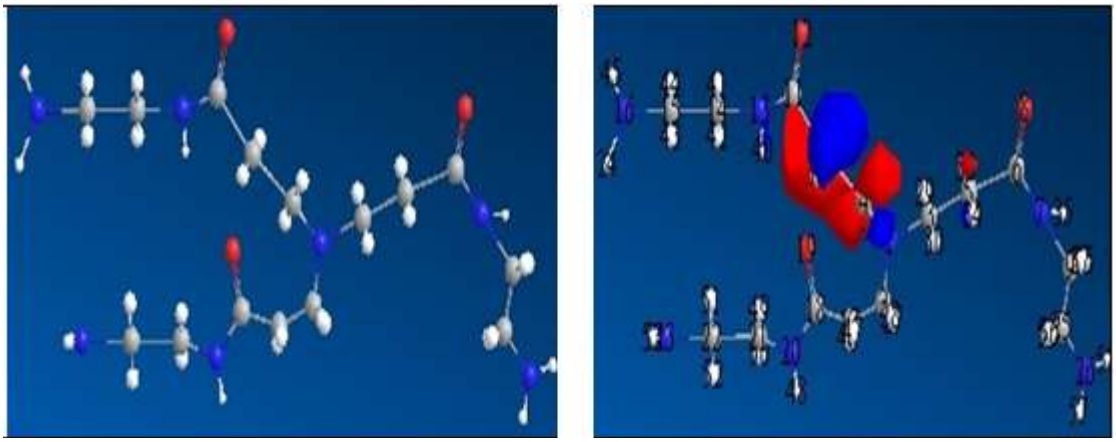

Figure 2: Equilibrium geometry for dendrimer (G1) (PMMA) applying G03 program

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 maim 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
C_4-H_{30}	1.113
C_4-H_{31}	1.113
C_5-C_6	1.509
C_5-H_{32}	1.113
C_5-H_{33}	1.113
C_6-N_7	1.369
C_6-O_8	1.208
N_7-C_9	1.460
N_7-H_{34}	1.022
C_9-C_{24}	1.523
C_9-H_{35}	1.113
C_9-H_{36}	1.113
C_{10}-C_{11}	1.509
C_{10}-H_{37}	1.113
C_{10}-H_{38}	1.113
C_{11}-O_{12}	1.208
C_{11}-N_{13}	1.369
N_{13}-C_{14}	1.460
N_{13}-H_{39}	1.022
C_{14}-C_{15}	1.523
C_{14}-H_{40}	1.113
C_{14}-H_{41}	1.113
C_{15}-N_{16}	1.468
C_{15}-H_{42}	1.113
C_{15}-H_{43}	1.113
N_{16}-H_{44}	1.035
N_{16}-H_{45}	1.035
N_{16}-Lp_{60}	0.600
C_{17}-C_{18}	1.509
C_{17}-H_{46}	1.113
C_{17}-H_{47}	1.113
C_{18}-O_{19}	1.208
C_{18}-N_{20}	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°

C_{14}-N_{13}-H_{39}	118.000°
N_{13}-C_{14}-C_{15}	109.280°
C_{15}-C_{14}-H_{40}	109.410°
C_{15}-C_{14}-H_{41}	109.410°
H_{40}-C_{14}-H_{41}	109.400°
C_{14}-C_{15}-N_{16}	109.500°
C_{14}-C_{15}-H_{42}	109.410°
C_{14}-C_{15}-H_{43}	109.410°
H_{42}-C_{15}-H_{43}	109.400°
H_{44}-N_{16}-H_{45}	104.500°
C_{2}-C_{17}-C_{18}	110.000°
C_{2}-C_{17}-H_{46}	109.410°
C_{2}-C_{17}-H_{47}	109.410°
C_{18}-C_{17}-H_{46}	108.800°
C_{18}-C_{17}-H_{47}	108.800°
H_{46}-C_{17}-H_{47}	109.400°
C_{17}-C_{18}-O_{19}	122.500°
C_{7}-C_{18}-N_{20}	114.000°
O_{19}-C_{18}-N_{20}	122.600°
C_{18}-N_{20}-H_{48}	117.400°
C_{21}-N_{20}-H_{48}	118.000°
N_{20}-C_{21}-C_{22}	109.280°
C_{22}-C_{21}-H_{49}	109.410°
C_{22}-C_{21}-H_{50}	109.410°
H_{49}-C_{21}-H_{50}	109.400
C_{21}-C_{22}-N_{23}	109.500°
C_{21}-C_{22}-H_{51}	109.500°
C_{21}-C_{22}-H_{52}	109.410°
H_{51}-C_{22}-H_{52}	109.410°
H_{53}-N_{23}-H_{54}	109.400°
C_{9}-C_{24}-N_{25}	104.500°
C_{9}-C_{24}-H_{55}	109.500°
C_{9}-C_{24}-H_{56}	109.410°
H_{55}-C_{24}-H_{56}	109.400°
H_{57}-N_{25}-H_{58}	104.500°

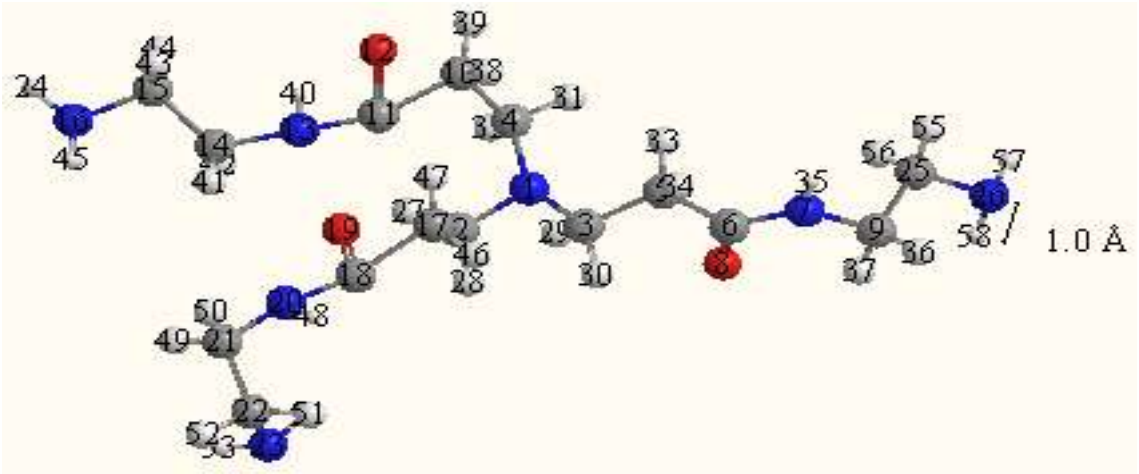

Figure 3: Repetitious section of the bonds and angles of *Dendrimers (PMMA.)* at their equilibrium geometries

Fundamental vibrations of Dendrimers (PMMA) were calculated and assigned like rocking modes (table 4), CH twisting modes, scissoring mode, CH wagging mode, γ NH, (O=C-- N)str and CHstr. The Dendrimers (PMMA), own 168 basic vibrations. scrutiny of the irreducible representations model, is definite by the table of symmetry character. Vibrational frequencies modes in the table are sorted in agreement with the Herzberg scheme [18]. Expose (table 4.) the computed vibrational frequencies modes and intensities of IR values to dendrimers G1 (PMMA).

4. Classification of vibration frequencies of (PMMA)

In-plane modes deformation vibrations frequencies δCH2 .

The calculated vibrations frequencies values were about (11.642-595.289 cm-1). as shown in (table-4).

Out-plane modes deformation vibrations frequencies (γNH) .

The calculated vibrations frequencies values were about (50.063-98.102 cm^{-1}). as shown in (table-4).

The CH stretching vibration

The calculated vibrations frequencies values were about (3178.317- 3935.579 cm^{-1}). as shown in (table-4).

The (O=C-N) stretching vibration

The calculated vibrations frequencies values were about (2138.660- 2167.040 cm^{-1}). as shown in (table-4). The IR. Absorption intensities values were about (370.185-0.259) Km mol^{-1} as shown in (table- 4). Analysis of IR absorption of (PMMA) has been well consolidated [19,20]. Also, the new inquiry into the vibrational motion modes and common coordinate analysis yielded a complete and extremely clear data on the basic vibrations of (PMMA) system [21]. The

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].

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

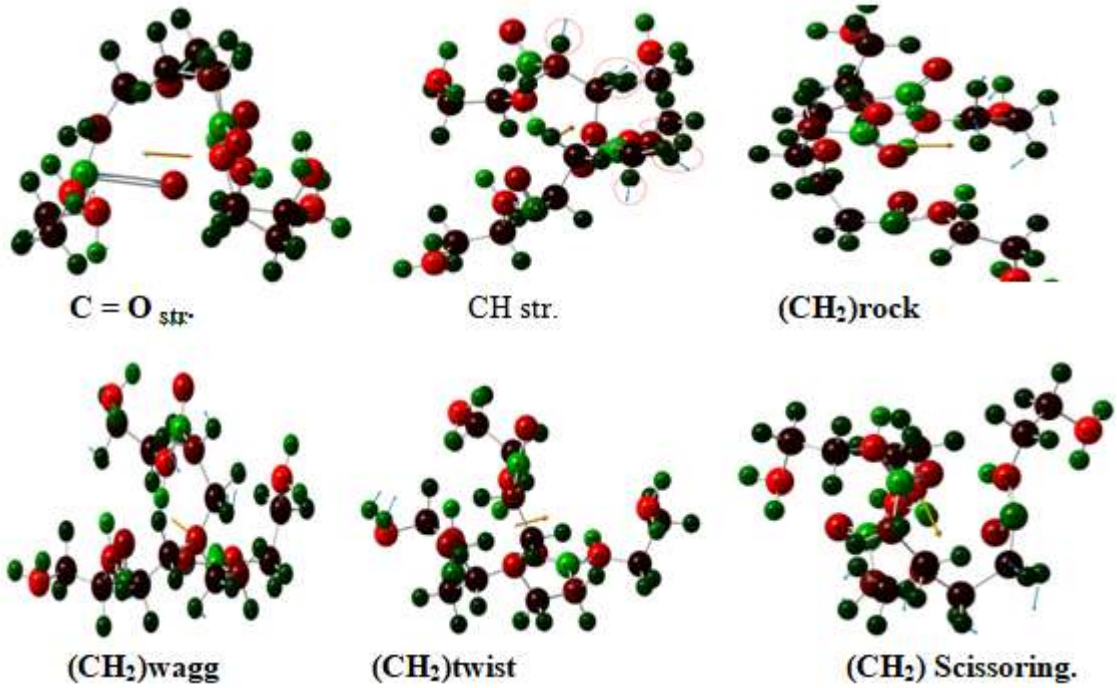

Figure 4: The graphical pictures of some vibration modes for Dendrimers (PMMA) calculated applying G03 program

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

Symmetry and description		*Frequency cm-1*	Intensity km/mol
ν_1	ρ(CH_2)rock	11.642	0.718
ν_2	ρ(CH_2)rock	16.556	1.990
ν_3	ρ(CH_2)rock	17.904	1.141
ν_4	ρ(CH_2)rock	26.567	0.311
ν_5	ρ(CH_2)rock	30.752	1.473
ν_6	ρ(CH_2)rock	39.834	1.176
ν_7	γ NH	50.063	1.668
ν_8	γ NH	55.241	2.462
ν_9	γ NH	61.382	10.201
ν_{10}	γ NH	71.745	0.254
ν_{11}	γ NH	87.196	2.852
ν_{12}	γ NH	98.102	4.472
ν_{13}	δ(CH)	106.924	1.422
ν_{14}	ρ(CH_2) rock	118.263	2.144
ν_{15}	ρ(CH_2) rock	120.493	0.259
ν_{16}	ρ(CH_2) rock	131.048	1.817
ν_{17}	ρ(CH_2) rock	161.344	4.312
ν_{18}	ρ(CH_2) rock	173.341	4.472
ν_{19}	ρ(CH_2) rock	184.212	40.631
ν_{20}	ρ(CH_2) rock	193.175	13.123
ν_{21}	ρ(CH_2) rock	206.737	7.226
ν_{22}	ρ(CH_2) rock	219.145	21.327
ν_{23}	ρ(CH_2) rock	229.048	6.267
ν_{24}	ρ(CH_2) rock	249.654	8.218
ν_{25}	ρ(CH_2) rock	263.727	2.955
ν_{26}	ρ(CH_2) rock	271.742	35.447
ν_{27}	ρ(CH_2) rock	291.743	13.247
ν_{28}	ρ(CH_2) rock	296.291	2.259
ν_{29}	ρ(CH_2) rock	316.406	1.811
ν_{30}	ρ(CH_2) rock	328.122	68.865
ν_{31}	ρ(CH2) rock	337.764	4.398
ν_{32}	ρ(CH2) rock	357.034	2.483
ν_{33}	ρ(CH2) rock	392.502	2.318
ν_{34}	ρ(CH2) rock	406.355	16.017
ν_{35}	ρ(CH2) rock	413.256	3.099
ν_{36}	ρ(CH2) rock	460.790	1.723
ν_{37}	τ(CH2) twist.	489.287	24.112
ν_{38}	ρ(CH2) rock	495.483	39.570
ν_{39}	ρ(CH2) rock	529.209	3.365
ν_{40}	ρ(CH2) rock	530.947	1.406
ν_{41}	ρ(CH2) rock	560.760	27.551
ν_{42}	ρ(CH2) rock	571.037	10.491
ν_{43}	ρ(CH2) rock	595.289	6.840
ν_{44}	ω(CH2).wagging	608.167	33.969
ν_{45}	ω(CH2).wagging	610.457	185.400
ν_{46}	ω(CH2).wagging	640.587	134.341
ν_{47}	ω(CH2).wagging	658.462	15.376
ν_{48}	ω(CH2).wagging	689.015	7.247
ν_{49}	ω(CH2).wagging	709.448	370.185

ν_{50}	τ(CH2)twist.	746.686	21.713
ν_{51}	ρ(CH_2)rock.	765.661	173.990
ν_{52}	ρ(CH_2)rock.	786.476	168.311
ν_{53}	τ(CH_2)twist.	808.642	25.282
ν_{54}	τ(CH_2)twist.	855.063	75.859
ν_{55}	τ(CH_2)twist.	871.786	72.725
ν_{56}	τ(CH_2)twist.	886.543	8.061
ν_{57}	τ(CH_2)twist.	889.161	0.723
ν_{58}	τ(CH_2)twist.	930.465	14.750
ν_{59}	τ(CH_2)twist.	936.438	8.885
ν_{60}	τ(CH_2)twist.	951.827	87.485
ν_{61}	ρ(CH_2)rock.	974.548	101.131
ν_{62}	τ(CH_2)twist.	987.600	2.442
ν_{63}	ρ(CH_2)rock.	1004.496	30.824
ν_{64}	τ(CH_2)twist.	1006.189	3.502
ν_{65}	ρ(CH_2)rock.	1031.610	3.357
ν_{66}	ρ(CH_2)rock.	1053.167	7.873
ν_{67}	ρ(CH_2)rock.	1071.139	3.527
ν_{68}	τ(CH_2)twist.	1074.475	9.158
ν_{69}	τ(CH_2)twist.	1090.646	18.629
ν_{70}	ρ(CH_2) rock.	1117.454	13.486
ν_{71}	τ(CH_2)twist.	1124.143	24.404
ν_{72}	τ(CH_2)twist.	1152.310	64.709
ν_{73}	τ(CH_2)twist.	1157.813	34.449
ν_{74}	τ(CH_2)twist.	1162.972	71.317
ν_{75}	τ(CH_2)twist.	1190.700	35.262
ν_{76}	τ(CH_2)twist.	1195.607	9.062
ν_{77}	ω(CH_2)wagg.	1200.976	36.855
ν_{78}	ω(CH_2)wagg.	1214.970	44.133
ν_{79}	ω(CH_2)wagg.	1217.243	111.358
ν_{80}	ω(CH_2)wagg.	1224.316	245.251
ν_{81}	ω(CH_2)wagg.	1234.615	7.147
ν_{82}	ω(CH_2)wagg.	1239.484	10.722
ν_{83}	τ(CH_2)twist.	1266.367	72.500
ν_{84}	τ(CH_2)twist.	1273.535	15.538
ν_{85}	τ(CH_2)twist.	1283.974	58.970
ν_{86}	τ(CH_2)twist.	1300.802	1.779
ν_{87}	τ(CH_2)twist.	1314.509	16.547
ν_{88}	τ(CH_2)twist.	1321.052	1.172
ν_{89}	τ(CH_2)twist.	1374.669	25.868
ν_{90}	τ(CH_2)twist.	1383.675	9.508
ν_{91}	τ(CH_2)twist.	1404.073	57.251
ν_{92}	τ(CH_2)twist.	1411.474	53.863
ν_{93}	τ(CH_2)twist.	1420.327	80.967
ν_{94}	τ(CH_2)twist.	1421.429	30.532
ν_{95}	τ(CH_2)twist.	1430.587	6.579
ν_{96}	τ(CH_2)twist.	1447.869	35.390
ν_{97}	τ(CH_2)twist.	1458.435	28.319
ν_{98}	τ(CH_2)twist.	1459.407	16.854
ν_{99}	τ(CH_2)twist.	1469.288	140.797
ν_{100}	ω(CH_2)wagg.	1475.473	1.740
ν_{101}	ω(CH_2)wagg.	1482.120	9.168
ν_{102}	τ(CH_2)twist.	1499.712	39.672
ν_{103}	ω(CH_2)wagg.	1500.388	37.110
ν_{104}	ω(CH_2)wagg.	1506.099	29.328
ν_{105}	ω(CH_2)wagg.	1523.698	6.370
ν_{106}	ω(CH_2)wagg.	1544.017	33.274
ν_{107}	ω(CH_2)wagg.	1547.495	4.304
ν_{108}	ω(CH_2)wagg.	1550.786	19.277
ν_{109}	ω(CH_2)wagg.	1555.056	2.852
ν_{110}	ω(CH_2)wagg.	1563.202	4.510
ν_{111}	ω(CH_2)wagg.	1564.267	17.673
ν_{112}	ω(CH_2)wagg.	1570.310	12.878
ν_{113}	ω(CH_2)wagg.	1571.941	16.274
ν_{114}	ω(CH_2)wagg	1585.022	152.323
ν_{115}	ω(CH_2)wagg	1590.189	2.916
ν_{116}	ω(CH_2)wagg	1621.770	7.232
ν_{117}	ω(CH_2)wagg	1633.13 74	30.323
ν_{118}	ω(CH_2)wagg	1637.849	7.472
ν_{119}	ς(CH_2) Scissoring.	1641.624	2.380
ν_{120}	ς(CH_2) Scissoring.	1645.390	4.803
ν_{121}	ς(CH_2) Scissoring.	1656.773	7.359
ν_{122}	ς(CH_2) Scissoring.	1662.916	12.709
ν_{123}	ς(CH_2) Scissoring.	1665.468	10.563
ν_{124}	ς(CH_2) Scissoring.	1668.976	3.084
ν_{125}	ς(CH_2) Scissoring.	1670.219	8.130
ν_{126}	ς(CH_2) Scissoring.	1675.335	6.447
ν_{127}	ς(CH_2) Scissoring.	1676.179	5.647
ν_{128}	ς(CH_2) Scissoring.	1689.909	4.221
ν_{129}	ς(CH_2) Scissoring.	1708.164	278.366
ν_{130}	ς(CH_2) Scissoring.	1730.951	305.540
ν_{131}	ς(CH_2) Scissoring.	1833.449	307.972
ν_{132}	ς(NH_2) Scissoring.	1842.598	369.351
ν_{133}	ς(NH_2) Scissoring.	1846.376	48.229
ν_{134}	ς(NH_2) Scissoring.	1847.151	105.238
ν_{135}	ς(NH2) Scissoring.	1864.745	38.903
ν_{136}	(O=C-- N)str.	2138.660	135.966
ν_{137}	(O=C-- N)str.	2146.810	101.233
ν_{138}	(O=C-- N)str.	2167.040	38.657
ν_{139}	CH str.	3147.209	91.367
ν_{140}	CH str.	3156.575	49.615
ν_{141}	CH str.	3178.317	22.323
ν_{142}	CH str.	3185.021	71.395
ν_{143}	CH str.	3195.921	41.015
ν_{144}	CH str.	3202.411	23.342
ν_{145}	CH str.	3213.789	27.601
ν_{146}	CH str.	3214.915	28.417
ν_{147}	CH str.	3236.002	65.1639
ν_{148}	CH str.	3236.156	40.690
ν_{149}	CH str.	3251.477	38.258
ν_{150}	CH str.	3251.8646	32.477
ν_{151}	CH str.	3263.689	1.9762
ν_{152}	CH str.	3265.220	62.006
ν_{153}	CH str.	3268.588	12.801
ν_{154}	CH str.	3285.967	18.927
ν155	CH str.	3287.368	19.339
ν_{156}	CH str.	3290.557	18.025
ν_{157}	CH str.	3311.726	5.852
ν_{158}	CH str.	3312.830	10.441
ν_{159}	CH str.	3334.031	23.451
ν_{160}	CH str.	3778.925	23.910
ν_{161}	CH str.	3784.673	41.577
ν_{162}	CH str.	3794.293	3.432
ν_{163}	CH str.	3812.932	5.290
ν_{164}	CH str.	3827.793	158.537
ν_{165}	CH str.	3851.030	36.092
ν_{166}	CH str.	3905.931	42.072
ν_{167}	CH str.	3913.241	10.522
ν_{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 legths 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, γNH, (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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