

Simulating NMR Spectrum of $C_{120}O$ through ab Initio Method

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ABSTRACT: The NMR spectrum of $C_{120}O$ has been calculated through Ab Initio method. The simplest structure of $C_{120}O$ molecule has one hundred and twenty carbon nuclei while oxygen is atom attached with two carbon atoms of fullerene. The structure, $C_{120}O$ molecule shows C_1 symmetry. $C_{120}O$ gives 357 degree of freedom which includes all the translations and rotations of the molecule. The structures of $C_{120}O$ are very sensitive to electron correlation treatment with basis set so STO-3G (5D, 7F) basis set. The simulated NMR spectrum of taken model $C_{120}O$ contains one hundred and twenty one lines. The average simulation peak of $C_{120}O$ compared is 103.24 ppm.

KEYWORDS: C_{60} , NMR spectrum, $C_{60}O$, $C_{120}O$ and fullerene

I. INTRODUCTION

Dimeric fullerenes have attracted attention as models for fullerene polymers as well as compounds [1]. The direct linked of C_{60} cages preparation and characterization becomes an important frontier in fullerene chemistry [2]. These empty cages polymers have particular physical and chemical properties that have to determine. These conjugations of the carbon cage might make this breed of polymer which having the wide potential application in electronic device. Rao et al reported that the production of C_{60} polymers via $[2C_2]$ photo-cyclo-addition in a C_{60} film [3]. They related C_{60} film in this plasma polymerization [4]. It is found that C_{119} cluster has been discovered through mass spectrometry in both the photolysis of C_{60} and benzil [5, 6] with the thermal decomposition of $C_{60}O$ [7]. Taylor et al proposed the mechanism of generation of C_{119} , through thermal decarbonylation of $C_{60}O$. He also proposed the result from C_{59} to C_{60} [8]. They stated that that $C_{60}O$ and $C_{120}O$ could provide as an important pioneer of new fullerene derivatives. He found that $C_{120}O$ could be found by thermal reacted C_{60} with $C_{60}O$ [8, 9]. He also recommended structure for $C_{120}O$ involves a direct bond between C_{60} units. The focus of the paper is to find NMR of $C_{120}O$.

II. MODEL

The initial structure of $C_{120}O$ was formed with the help of molecular mechanics (MM) such that the center of mass at the origin of coordinates. The intercage C–C bond structure of $C_{120}O$ is in direction parallel to the x-axis. This structure contains furan ring. The plane of the furan ring as the xy- plane as represented in Figure 1. The coordinates of all carbon atoms and oxygen atom are well connected as shown in the below figure. The structure of $C_{120}O$ contains two units of C_{60} . These two units C_{60} connect together produced the furan ring by the 6–6 bonds and the final optimized structure has almost two identical units. A symmetric plane is cut from the middle point of $C_{120}O$ through C(40)–C(93) bond and the oxygen atom formulate the two cages mirror each other. The other symmetric plane is perpendicular to the previous given above that divides the two cages into two almost identical halves, with the furan ring stretch out in this plane, so, $C_{120}O$ has C_{2v} symmetry. The optimal bond length and bond order of $C_{120}O$ are including all kinds of C–C bonds and one kind of C–O bond.

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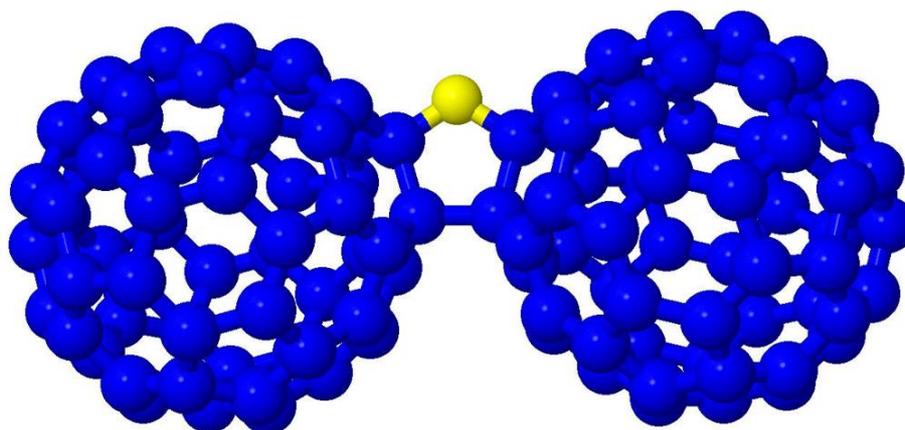


Figure 1 shows C₁₂₀O structure configurations

III. CALCULATIONS

Calculations of NMR shielding tensors have been published from many years [13-16]; these methods are all applicable to calculate the magnetic shielding function of different molecules. All the calculations of NMR have been done according to Rashid Nizam et al [20].

IV. RESULTS AND DISCUSSIONS

The fullerenes derivative, C₁₂₀O has 357 degree of freedom. Actually it starts with 180 total degrees of freedom for each an isolated C₆₀ molecule. Then subtracting the six degrees of freedom corresponding to three translations and three rotations, results in 354 vibrational degrees of freedom. Then finally add three rotations degree of freedom of oxygen to C₁₂₀ molecule which gives 357 degree of freedom. The rotational constants in x, y, and z axis in the fullerenes derivative (C₁₂₀O) is 0.04 0.01 and 0.01 (GHz) respectively. The C₁₂₀O has 605 symmetry adapted basis functions, 1815 primitive gaussians, 605 cartesian basis functions, 364 alpha electrons and 364 beta electrons with the nuclear repulsion energy 24579.43 Hartrees. The fullerenes derivative (C₁₂₀O) has done SCF E (RHF) = -4562.37 A.U. after 16 cycles with convergence density matrix= 0.5141D-08

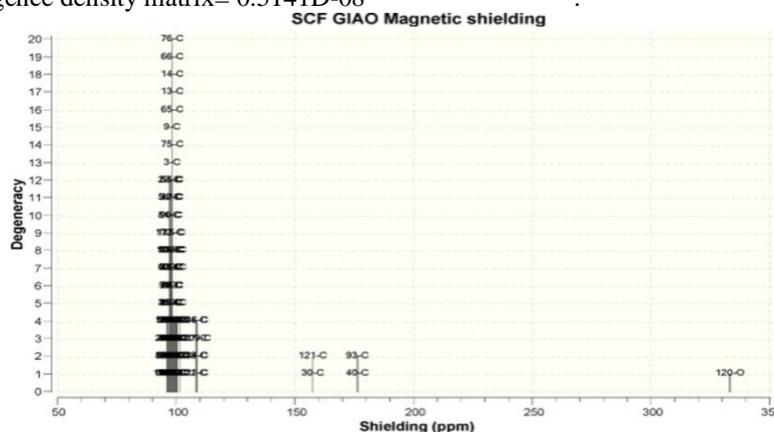


Figure 2 shows NMR of C₁₂₀O

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Mostly NMR experiment, any $C_{120}O$ molecules having the distribution of ^{12}C to ^{13}C isotopes is in proportion to 75 to 25 percent. Therefore about more than half of the molecules in $C_{120}O$ samples experiment are $^{12}C_{120}O$ molecules, which do not give NMR spectrum. Still the isotope effects discussed above are expected to influence the line intensities of the rotational and rotational-vibrational modes significantly in ordinary $C_{120}O$ samples at very low temperatures. The simulated NMR spectrum of model $C_{120}O$ contains one hundred and twenty one lines as shown in figure 2. In $^{13}C_{120}O$, each ^{13}C atom and ^{17}O has a nuclear spin $\phi = 1/2$ and each molecule of $^{13}C_{120}O$ thus has 2^{121} nuclear spin states, with ϕ_{tot} values ranging from $\phi_{tot} = 0$ to $\phi_{tot} = 121$. The statistical weight for each irreducible representation of C or O for all 2^{121} states of $^{13}C_{120}O$ is well approximated by the dimension of the irreducible representation. The NMR simulated peaks of $^{13}C_{120}O$ model are given below. The number in the bracket represents the number of NMR peaks obtaining at particular atom $^{13}C_{120}O$.

In detail, the calculated NMR peaks shifts of $C_{120}O$ are as follows (in ppm.): 96.19(1 C), 97.57(2C), 98.43(3C), 98.4398.43(4C), 99.50(5C), 98.42(6C), 100.43(7C), 97.01(8C), 98.44(8C), 98.422(9C), 98.11(10C), 97.71(12C), 98.44(13C), 98.44(14C), 99.52(15C), 98.42(16C), 101.66(17C), 108.23(18C), 97.00(19C), 98.28(20C), 100.30(21C), 108.95(22C), 97.04(23C), 98.09(24C), 97.40(25C), 97.71(26C), 97.57(27C), 96.19(28C), 101.66(29C), 157.45(30C), 96.59(31C), 97.81(32C), 97.76(33C), 97.42(34C), 98.11(35C), 97.01(36C), 108.22(37C), 100.43(38C), 99.20(39C), 176.59(40C), 98.51(41C), 98.43(42C), 98.50(43C), 100.03(44C), 99.20(45C), 108.96(46C), 97.00(47C), 98.28(48C), 97.76(49C), 98.09(50C), 98.62(51C), 98.50(52C), 100.30(53C), 97.04(54C), 98.43(55C), 96.59(56C), 97.82(57C), 98.52(58C), 98.62(59C), 100.02(60C), 97.57(61C), 96.18(62C), 99.51(63C), 98.41(64C), 98.44(65C), 98.44(66C), 97.01(67C), 100.42(68C), 98.42(69C), 98.42(70C), 108.21(71C), 101.65(72C), 98.43(73C), 99.50(74C), 98.43(75C), 98.44(76C), 97.71(77C), 98.11(78C), 98.28(79C), 97.00(80C), 97.03(81C), 98.20(82C), 100.30(83C), 108.95(84C), 101.66(85C), 96.19(86C), 97.57(87C), 97.71(88C), 97.40(89C), 97.81(90C), 96.58(91C), 99.20(92C), 176.59(93C), 108.23(94C), 100.43(95C), 98.11(96C), 97.01(97C), 97.76(98C), 97.42(99C), 100.02(100C), 98.50(101C), 98.42(102C), 98.51(103C), 97.76(104C), 98.09(105C), 98.28(106C), 97.00(107C), 99.20(108C), 108.95(109C), 98.63(110C), 98.42(111C), 97.03(112C), 100.30(113C), 98.50(114C), 97.80(115C), 96.57(116C), 100.03(117C), 98.61(118C), 98.50(119C), 333.12(121O), 157.45(120C)

The average of simulated NMR of $C_{120}O$ is at 103.24 ppm. We have not found any simulated or experimental NMR data of $C_{120}O$ molecule on the internet. If compared with the observed NMR data peak with our simulated NMR of $^{13}C_{120}O$ then they may give slightly different NMR data. This may be due to two reasons.

First, the entire experimental sample $^{13}C_{120}O$ might not possess all ^{13}C and ^{17}O during the NMR experiment. While the simulated structure of $^{13}C_{120}O$ presenting one hundred and twenty one lines or peaks because the entire model contains ^{13}C and ^{17}O isotopes.

Second, measured experimentally is the difference in resonance frequency between the NMR of $^{13}C_{120}O$ and that of a reference compound which containing the nuclear species being studied. Generally insulators are taken as the reference compound, since they have zero Knight shift. However, these insulators do, have chemical shifts relative to a hypothetical bare nucleus. Therefore the measured shifts relative to a reference compound represent the sum of the Knight shift plus the chemical shift relative to the reference compound. It is very difficult to deduce the separate contributions of the Knight- shift from chemical-shift terms.

V. CONCLUSION

The structures of $C_{120}O$ are very sensitive to electron correlation treatment with basis set that are used. In this paper we have used STO-3G (5D, 7F) basis set. The simulated NMR spectrum of taken model $C_{120}O$ contains one hundred and twenty one lines. The average simulation peak of $C_{120}O$ compared is 103.24 ppm.

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