

# Time-Resolved EPR and Fourier Transform EPR Study of Triplet C<sub>60</sub>. Determinations of T<sub>1</sub> and the <sup>13</sup>C Hyperfine Coupling Constant

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Continuous wave (CW) and time-resolved (TR) EPR spectra of triplet C<sub>60</sub> with partial and full <sup>13</sup>C enrichment in methylcyclohexane solutions after UV irradiation were obtained. Line broadening from <sup>13</sup>C satellites was observed. The <sup>13</sup>C hyperfine coupling constant was determined to be 0.06 G. Fourier transform EPR (FT-EPR) experiments with a resolution of 20 ns were carried out, and T<sub>1</sub> was found to be 0.8 ± 0.1 μs by fitting the intensity of the free induction decay signal to the modified Bloch equations. The relaxation time from FT-EPR is in excellent agreement with estimations from the line width of CW-EPR. Because the <sup>13</sup>C hyperfine coupling constant is so small, no distinct satellite lines were observed with <sup>13</sup>C in natural abundance at 200 K.

In a previous paper,<sup>1</sup> the continuous wave (CW) and time-resolved (TR) EPR spectra obtained by UV irradiation of methylcyclohexane solution of C<sub>60</sub> were reported. A single sharp, approximately Lorentzian, absorption line with a peak-to-peak line width of 0.14 G was observed at room temperature. This EPR spectrum was assigned to the lowest triplet state of C<sub>60</sub> (<sup>3</sup>C<sub>60</sub>). The narrow line width was attributed to a very rapid interchange of the magnetic axes by pseudorotation, switching the degenerate Jahn-Teller states into each other. However, "an unresolved mystery" remained at that time since no <sup>13</sup>C satellites were observed. Since the probability for a C<sub>60</sub> molecule to contain no <sup>13</sup>C atoms is 51%, the possibility that <sup>13</sup>C might be a very efficient quencher of <sup>3</sup>C<sub>60</sub>, thus reducing the lifetime of <sup>3</sup>C<sub>60</sub> to less than 1 μs, existed. Therefore, TR-EPR spectra taken 1 μs after laser excitation of C<sub>60</sub> would not show any hyperfine structure. In this paper, the "mystery" is resolved by studying CW- and TR-EPR spectra of triplet C<sub>60</sub> with partial and full <sup>13</sup>C enrichment. In addition, the hyperfine coupling constant for <sup>13</sup>C was determined from these spectra.

The synthesis of <sup>13</sup>C<sub>60</sub> and experimental procedures and conditions for both the CW- and the TR-EPR measurements were described in previous papers.<sup>1,2</sup> As shown in Figure 1, both the partially (25%) and fully (99%+) <sup>13</sup>C-enriched C<sub>60</sub> triplets produce a broadened absorption spectrum compared with that of the unenriched one, with a line width of 0.28 and 0.45 G, respectively, vs the natural abundance line width of 0.16 G at 200 K. Figure 2 shows the TR-EPR spectra of 25% <sup>13</sup>C-enriched C<sub>60</sub> at various times after the laser excitation. Weak satellites are present. The absorption intensity decreases as <sup>3</sup>C<sub>60</sub> decays, giving an estimated lifetime of about 30 μs. However, the line width and the shape of the absorption remain unchanged throughout the observation time. This is strong evidence against the previous suspicion that <sup>13</sup>C might be an efficient quencher of <sup>3</sup>C<sub>60</sub>. Also, flash photolysis experiments were repeated on the 25% <sup>13</sup>C-

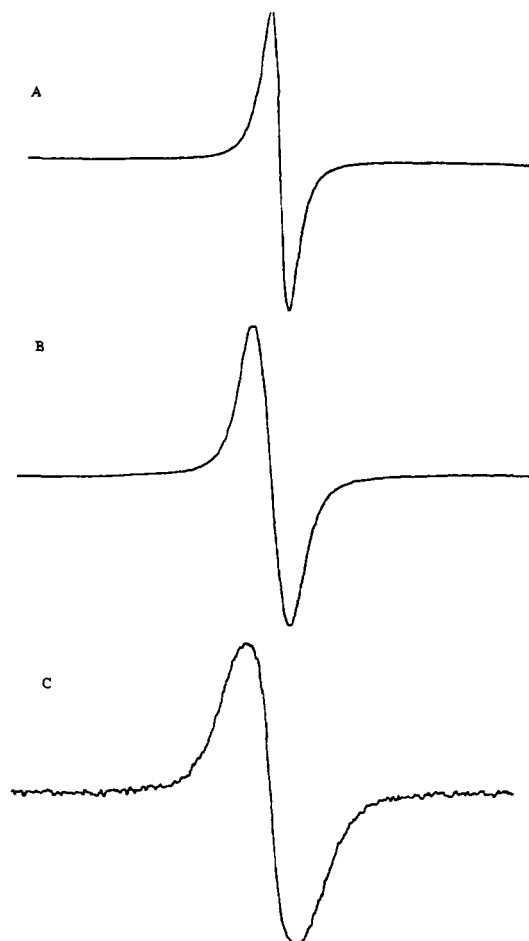
enriched C<sub>60</sub> sample, resulting in the same lifetime as reported previously for the unenriched sample.<sup>1,3-7</sup> The EPR spectrum of <sup>3</sup>C<sub>60</sub> with <sup>13</sup>C in natural abundance has an approximately Lorentzian line shape, while that of the 99% + <sup>13</sup>C-enriched <sup>3</sup>C<sub>60</sub> has an approximately Gaussian shape. For the 25% enriched <sup>3</sup>C<sub>60</sub>, the line shape is neither Lorentzian nor Gaussian, but a combination of the two (Figure 3).

Debates on whether this photogenerated paramagnetic species is <sup>3</sup>C<sub>60</sub> or the C<sub>60</sub> radical anion C<sub>60</sub><sup>-</sup>, or "a loose ion pair within an aggregate which consists of C<sub>60</sub> clusters, i.e. [C<sub>60</sub><sup>+</sup>, e<sup>-</sup>]",<sup>9</sup> exist at the present time. Dinse et al.<sup>8</sup> made the reasonable suggestion that the radical anion is responsible for the EPR spectra, partially because of the slow rise time of the signal intensity in the Fourier transform EPR (FT-EPR) experiments. Since the intersystem crossing process of C<sub>60</sub> is complete in several nanoseconds,<sup>4,10-14</sup> a long rise time of 1 μs may disallow the assignment of the species to a triplet state. However, this argument needs to be not true. The dictum that the intensity of an EPR spectrum is proportional to the population difference of the two energy levels does not necessarily hold during the formation and decay of spin magnetization. For observations made at times as short as several nanoseconds, the signal intensity does not necessarily reflect the populations of the two spin states. Instead, the EPR intensity requires additional time to reach the maximum value. This "induction" period has a value close to that of T<sub>1</sub> and also depends on the lifetime of the paramagnetic species and spin polarization mechanism.

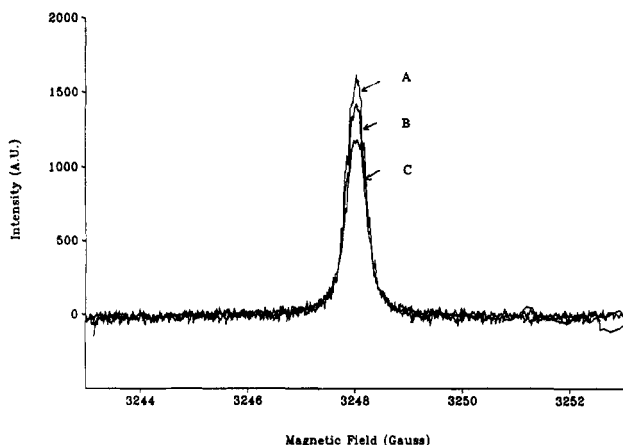
We repeated the FT-EPR experiments performed by Dinse and co-workers<sup>8</sup> at 197 K, with a resolution of 20 ns, on both normal and the 25% <sup>13</sup>C-enriched C<sub>60</sub> in methylcyclohexane solution. We also found that the signal intensity grows slowly and reaches a maximum at about 2 μs after laser excitation (Figure 4). Both samples show exactly the same rise and decay pattern. Fessenden carried out a detailed study of the intensity time profiles of the TR-EPR spectroscopy with CIDEP phenomena in the 1970s.<sup>15-18</sup> Here, we briefly describe the theoretical approach extended to the <sup>3</sup>C<sub>60</sub> system.

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**Figure 1.** Field-modulated CW-EPR signal of C<sub>60</sub> in methylcyclohexane irradiated with a xenon lamp: (a) natural abundance (1.1%) <sup>13</sup>C, with  $\Delta H_{\text{peak-to-peak}} = 0.14$  G; (b) 25% <sup>13</sup>C, with  $\Delta H_{\text{peak-to-peak}} = 0.28$  G; (c) 99%+ <sup>13</sup>C, with  $\Delta H_{\text{peak-to-peak}} = 0.45$  G.



**Figure 2.** Direct detection signal from TR-EPR of 25% <sup>13</sup>C-enriched <sup>3</sup>C<sub>60</sub> in methylcyclohexane solution at 203 K: (a) 8 μs, (b) 14 μs, (c) 25 μs after laser flash (308 nm).

The time evolution of the magnetic moment along the Z axis may be written as

$$\dot{M}_z + \frac{M_z}{T_1} + \frac{M_z}{T_c} = \frac{M_0}{T_1} e^{-t/T_c} [1 + kT_c M_0 (1 - e^{-t/T_c})] \quad (1)$$

where  $M_z$  is the magnetic moment in the rotating frame,  $T_1$  is the spin-lattice relaxation time, and  $M_0$  is the equilibrium magnetization at infinite time if the triplet excited state did not decay. The term  $M_0 e^{-t/T_c}$  represents the first-order decay of the triplet state to the singlet ground state via radiationless transition processes, where  $T_c$  is the lifetime of <sup>3</sup>C<sub>60</sub>. At high concentration,

another term responsible for the second-order decay of  $M_0$  should be included as the triplet-triplet annihilation process has been observed.<sup>3-5,11,14</sup> The rate constant  $k$  for this process is dependent on the concentration of ground-state C<sub>60</sub>, the temperature, and the laser power, and  $k$  is found to be around  $2 \times 10^9$  dm<sup>3</sup> mol<sup>-1</sup> s<sup>-1</sup> at room temperature with laser power at 1.5 mJ/pulse.<sup>14</sup> Equation 1 includes both decay processes.<sup>19</sup> At low concentration, when  $kT_c M_0 \ll 1$ , or at very short time, when  $(1 - e^{-t/T_c}) \rightarrow 0$ , this term can be approximated by  $M_0 e^{-t/T_c}$ . This simplification was used in solving the differential equation, and the solution for  $M_z$ , which is proportional to the signal intensity, is

$$M_z(t)_i = C_1 \exp[-(1/T_1 + 1/T_c)t] + C_2 P_i M_0 \times \exp(-t/T_c), \quad i = 1, 2 \quad (2)$$

where  $C_1$  and  $C_2$  are constants and  $P$  represents the degree of polarization, with a positive value for enhanced absorption and a negative one for emission.  $P_1$  and  $P_2$  are the polarization parameters for the two  $\Delta m = 1$  transitions in the triplet state. The averaged EPR spectrum in liquid solution is the sum of the two transition intensities, namely,  $M_z(t)_1 + M_z(t)_2$ . The final form of  $M_z(t)$  is described by eq 3

$$M_z(t) = A e^{-t/T_c} + B e^{-(1/T_1 + 1/T_c)t} \quad (3)$$

$T_1$  is found to be  $0.8 \pm 0.1$  μs by fitting the FT-EPR absorption data at different pulse delay time with eq 3 (Figure 4).<sup>20</sup> The temperature dependence of the rise time, which has been observed,<sup>8</sup> is expected from eq 3, as both  $T_c$  and  $T_1$  are temperature dependent. From the line width of the TR-EPR spectrum at room temperature and the expression for dipole-dipole-induced relaxation rates,<sup>21</sup> together with the experimental zero-field splitting parameters for <sup>3</sup>C<sub>60</sub>,<sup>11</sup>  $T_2$  is estimated to be 0.81 μs.<sup>11</sup> Therefore,  $T_1$  is found to be equal to  $T_2$  within experimental error from two different experiments. This equality was also reported by Dinse et al.<sup>8</sup>

The fact that  $T_1 = T_2$  indicates an extremely short rotational correlation time  $\tau_c$ , which we estimated to be between  $10^{-12}$  and  $10^{-13}$  s.<sup>1</sup> Such correlation times are considerably shorter than that observed for the classical rotation of ground-state C<sub>60</sub> in solution ( $\sim 10^{-11}$  s)<sup>22</sup> and support the proposal that the averaging of the zero-field anisotropy of <sup>3</sup>C<sub>60</sub> ( $D = 0.0114$  cm<sup>-1</sup>)<sup>11</sup> to produce a narrow absorption in methylcyclohexane solution of only 0.14 G at room temperature is due to a faster averaging process than classical rotation. This pseudorotation is the rapid switching of the magnetic axes (principal axes of the zero-field splitting tensor) within the molecule as a result of the rapid interconversion between degenerate Jahn-Teller distorted states caused by the degeneracy of the lowest electronic triplet state of C<sub>60</sub>.<sup>23</sup>

In order to quantitatively determine the hyperfine coupling constant between <sup>13</sup>C and the unpaired electrons in triplet C<sub>60</sub>, a mathematical model described by eq 4

$$\text{intensity} = \sum_{m=0}^{60} \sum_{n=0}^m P_{60}^m (1-x)^{60-m} x^m P_m^n Y_{10}^n / 2^m \quad (4)$$

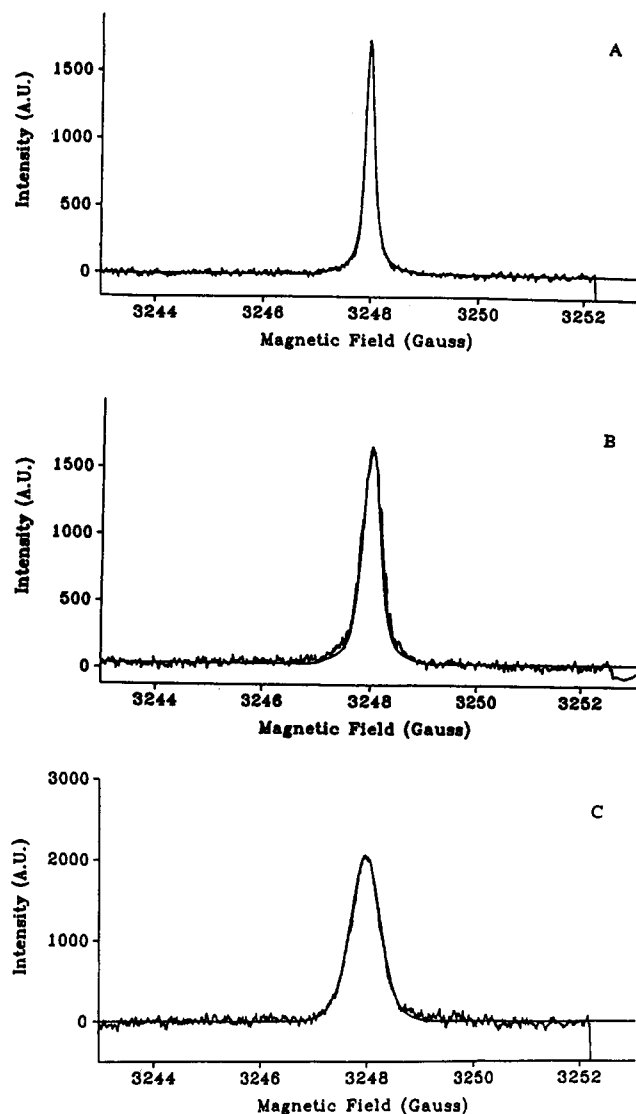
is used to simulate the absorption spectra obtained from the TR-EPR measurements. Here,  $x$  is the percentage of <sup>13</sup>C in the C<sub>60</sub> sample, and

$$P_{60}^m = 60 \cdot 59 \cdot 58 \cdots / m!$$

where  $m$  is the number of <sup>13</sup>C atoms in one C<sub>60</sub> molecule. The EPR spectrum for C<sub>60</sub> molecules containing  $m$  <sup>13</sup>C atoms has  $m + 1$  lines evenly separated by the hyperfine coupling constant. The intensities obey the binomial distribution of  $P_m^n$

$$P_m^n = m \cdot (m-1) \cdot (m-2) \cdots / n!$$

where  $n$  has values between 0 and  $m$  and denotes the  $n$ th hyperfine component counting from the left. The parameter  $Y_{10}$  is the



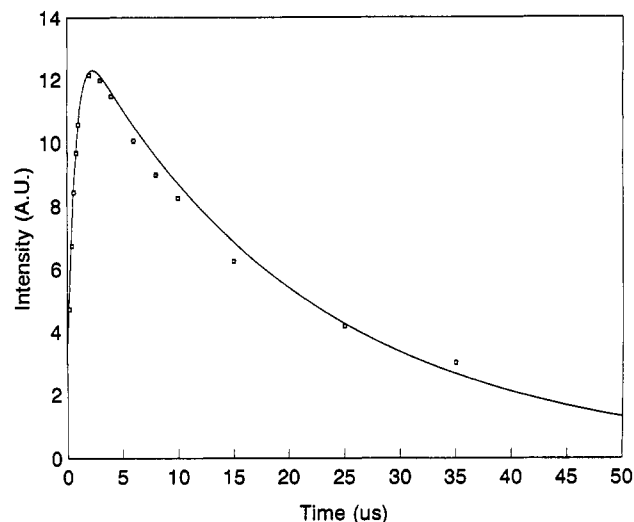
**Figure 3.** TR-EPR absorption spectra of (a) 1.1%  $^{13}\text{C}$ , (b) 25%  $^{13}\text{C}$ , and (c) 99%+  $^{13}\text{C}$ , and simulations with the hyperfine coupling constant equal to 0.06 G and a fwhm of 0.175 G.

expression for a Lorentzian line for the absorption intensity as a function of the magnetic field described by eq 5

$$Y_{10} = y_m / \{1 + [(H - (n-m/2)a_c) / \Delta H_{1/2}]^2\} \quad (5)$$

where  $H$  is the magnetic field,  $a_c$  is the hyperfine coupling constant, and  $y_m$  denotes the maximum amplitude obtained at the center of the line when  $H = (n-m/2)a_c$ . The parameter  $y_m$  also serves as a proportionality constant while fitting the experimental spectrum. Finally,  $\Delta H_{1/2}$  is the full line width between half-magnitude points (fwhm).

The model considers the absorption line shape as the overlap of the hyperfine multiplets expected for each isotopomer with intensities that are proportional to the abundance of each isotopomer. The following simplifications are employed: (1) The spin density is evenly distributed over the 60 carbons by virtue of rapid averaging on the EPR time scale. (2) Each  $^{13}\text{C}$  atom has the same hyperfine coupling constant regardless of its position in the molecule. (3) All stick spectra are convoluted with the same Lorentzian line width. (4) The probability of having a certain number of  $^{13}\text{C}$  nuclei in each isotopomer is based on simple combinatorial statistics. The simplest case is that of 99%  $^{13}\text{C}$ -enriched  $\text{C}_{60}$ , for which there is essentially only one isotopomer which gives rise to a multiplet of 61 lines of binomial relative intensities.



**Figure 4.** FT-EPR rising and decay of the intensity as a function of time. Solid line is a fit for the experimental data to the equation  $y = Ae^{-t/T_c} + Be^{-(1/T_1 + 1/T_c)t}$ , where  $A = 14.0$ ,  $B = -11.0$ ,  $T_c = 21 \mu\text{s}$ , and  $T_1 = 0.83 \mu\text{s}$ .

The pseudorotation proposal for the  $\text{C}_{60}$  excited triplet state makes the first two simplifications reasonable. The third assumption is well supported by the finding from FT-EPR that  $^{13}\text{C}$ -enriched  $^{13}\text{C}$  has the same  $T_1$  as  $^{13}\text{C}$  in natural abundance and the significant line shape change according to the percentage of  $^{13}\text{C}$  in the sample.

Figure 4 shows that a single hyperfine coupling constant of 0.06 G and a single line width for each hyperfine component of 0.175 G adequately simulates the observed line shape for three different  $^{13}\text{C}$  enrichments. The coupling constant is smaller than the initial estimation of approximately 0.68 G based on the  $^{13}\text{C}$  hyperfine splitting in the methyl radical and the McConnell–Weissman relation.<sup>1,24</sup> This estimation neglects spin polarization effects. In  $^{13}\text{C}_{60}$ , every carbon atom is connected to three other carbon atoms. Due to negative spin densities induced by the three C–C  $\sigma$  bonds from the adjacent carbons, the splitting is better represented by the “modified” McConnell–Weissman relation

$$a_c = Q_1\rho_1 + Q_2(\rho_2 + \rho_3 + \rho_4) \quad (6)$$

where  $a_c$  is the  $^{13}\text{C}$  hyperfine coupling constant;  $Q_1$  and  $Q_2$  are proportionality constants, with  $Q_1$  positive and  $Q_2$  negative; and  $\rho_1$ ,  $\rho_2$ ,  $\rho_3$ , and  $\rho_4$  are the spin densities on a particular carbon and the three attached carbons.<sup>21</sup>

Since very little study has been done on the  $^{13}\text{C}$  coupling in  $\text{C}_{60}$  at the present time, no  $Q_1$  and  $Q_2$  values have been reported. A good estimation is also not easy, due to the global-like structure of the molecule. A crude estimation of  $Q_1$  and  $Q_2$  based on the  $^{13}\text{C}$  hyperfine coupling constants of methyl radical and the benzene anion molecules is  $Q_1/Q_2 = -41/12$ .<sup>25</sup> Applying this relationship of  $Q_1$  and  $Q_2$  to eq 6, along with the relation  $\rho_1 = \rho_2 = \rho_3 = \rho_4$ , which equals 1/60 of the spin density of methyl radical,  $a_c$  is calculated from eq 6 to be 0.083 G. Also, the  $Q_1$  and  $Q_2$  determined from the modified McConnell–Weissman relation, using the experimental  $^{13}\text{C}$  coupling constants of the anthracene anion and cation and the spin densities determined by the Hückel theory,<sup>26</sup> are 45.4 and  $-16.6$ , respectively. Using these two values,  $a_c$  for  $^{13}\text{C}_{60}$  is calculated to be 0.073 G. Both estimations of  $a_c$  are very close to the experimental coupling constant of 0.06 G determined from our model.

Finally, it should be noted that the EPR behavior of electrochemically or chemically generated  $\text{C}_{60}$  radical anion is very different from the EPR behavior of triplet  $\text{C}_{60}$  reported here. The line width of  $\text{C}_{60}^{\cdot-}$  is ca. 6 G at low temperatures (120 K)<sup>27–30</sup> and increases dramatically with temperature<sup>29,30</sup> (60–80 G at

300 K, depending on the environment). In solution, the line width may be too broad to allow detection at the available concentrations. Although the assignment of the narrow line to the triplet state of C<sub>60</sub> is compatible with all our results, other possible assignments are not eliminated. However, the assignment is completely consistent with the recent results reported by Levanon and co-workers<sup>31</sup> and by van Willigen and co-workers.<sup>32</sup>

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This paper is dedicated to Professor Gerhard L. Closs, one of the finest chemists in this century. His scientific achievements were outstanding and numerous, including the establishment of chemically induced dynamic nuclear polarization, contributions to chemically induced electron polarization, and seminal studies of carbenes and other ground-state triplet species. His elegant experimental designs in studying electron-transfer reaction, together with John Miller, unambiguously demonstrated the existence of the Marcus inverted region proposed by Rudy Marcus, who received this year's Nobel Prize in chemistry. His sudden death is a great loss for chemistry. We would like to dedicate this paper to his memory, because the C<sub>60</sub> study was one of his many projects at the time of his death, and the "unresolved mystery" of the missing <sup>13</sup>C hyperfine splittings remained at that time. This paper is a continuation of his study on the excited triplet state of C<sub>60</sub>.

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- For a methyl radical, the <sup>13</sup>C hyperfine coupling constant, according to the McConnell–Weissman relation,  $a_c' = Q_1 \rho_1' = 41$  G (see ref 19). For benzene anions, due to equal negative spin densities contributed from the adjacent two C–C σ bonds, the modified McConnell–Weissman relation is  $a_c'' = Q_1 \rho_1'' + Q_2 (\rho_2'' + \rho_3'')$ , and  $a_c'' = 2.8$  G. Using the relation  $\rho_1'' = \rho_2'' = \rho_3'' = 1/6 \rho_1'$ ,  $Q_1/Q_2 = -41/12$ .
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