

Isotope Abundances of Fullerenes.

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The amount of Isotopic variations of the Fullerenes can be calculated ie ;

$$A = (P_{C_{12}})^{n-r} \cdot (P_{C_{13}})^r \cdot {}^nC_r$$

where A is abundance probability for isotope type ${}^{12}C_n {}^{13}C_r$

$P_{C_{12}}$ is natural abundance of C^{12} (0.98893)

$P_{C_{13}}$ " " " " C^{13} (0.01107)

nC_r is no of combinations of isomer ${}^{12}C_n {}^{13}C_r$

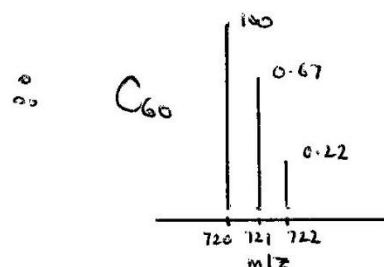
$${}^nC_r = \frac{n!}{r!(n-r)!}$$

For C_{60} :

$${}^{12}C_{60} {}^{13}C_0 \quad A_1 = (0.98893)^{60} \cdot (1)(1) = 0.513$$

$${}^{12}C_{59} {}^{13}C_1 \quad A_2 = (0.98893)^{59} \cdot (0.01107)^1 \cdot 60 = 0.344$$

$${}^{12}C_{58} {}^{13}C_2 \quad A_3 = (0.98893)^{58} \cdot (0.01107)^2 \cdot \frac{60 \cdot 59}{2} = 0.1137$$



Normalised
1.0
0.67
0.22

No of ^{13}C	Abundance	Relative Abundance
$^{12}\text{C}_{60}$	0.513	1.00
$^{12}\text{C}_{59}^{13}\text{C}_1$	0.344	0.67
$^{12}\text{C}_{58}^{13}\text{C}_2$	0.1137	0.22
$^{12}\text{C}_{70}$	0.459	1.00
$^{12}\text{C}_{69}^{13}\text{C}_1$	0.360	0.78
$^{12}\text{C}_{68}^{13}\text{C}_2$	0.139	0.30

These are from my PhD notes ca. August 1992

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