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Radical Recombination in γ -Irradiated Anthracene[†]

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Recent studies of electron paramagnetic resonance in γ -irradiated anthracene¹⁻⁴ indicate that the origin of the EPR signal is a radical in which the unpaired electron is coupled to three nearly equivalent protons. Harrah and Hughes² and Inoue³ have proposed that the dibenzocyclohexadienyl radical, formed by the addition of one extra hydrogen atom to the 9 or 10 position of an anthracene molecule, gives rise to the observed spectrum. From the annealing kinetics of the EPR signal, McGhie *et al.*⁵ conclude that a bimolecular reaction is the dominant mechanism for radical recombination.

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We have analyzed, by gas chromatography, anthracene which had exposures up to 10^9 R of Co^{60} γ radiation. Several new substances were found in concentrations proportional to the radiation dose, some with molecular weights of at least twice that of anthracene. Only one major substance eluted prior to anthracene. This material was collected in milligram quantities on a preparatory gas chromatograph and identified by ultraviolet spectroscopy as dihydroanthracene. A concentration of $4 \times 10^{18}/\text{cm}^3$ was found after exposure to 1.0×10^9 R. Similar analysis after irradiated anthracene was annealed for 37 hours at 175°C , a time and temperature at which the EPR signal is greatly reduced, showed that the dihydroanthracene concentration had doubled to $8 \times 10^{18}/\text{cm}^3$ for 1.0×10^9 R.

These results suggest that dihydroanthracene is one of the principal reaction products of the bimolecular radical recombination observed by McGhie *et al.*⁵ We propose a reaction in which two dibenzocyclohexadienyl radicals combine to form one dihydroanthracene molecule and one anthracene molecule. This would produce a dihydroanthracene concentration equal to one half that of the original radical concentration. Since McGhie *et al.* observed about 10^{19} spins/ cm^3 following exposure to 10^9 R, the change in dihydroanthracene concentration of $4 \times 10^{18}/\text{cm}^3$ after annealing supports the proposed reaction. The dihydroanthracene observed before annealing was probably produced directly during the irradiation. Although some dihydroanthracene may have been formed by the radicals abstracting a hydrogen atom within the chromatograph, it is not believed that this process is significant because of the concentration increase after annealing.

The presence of compounds much heavier than anthracene in the gas chromatogram implies that the radiation is also producing damage more serious than hydrogen atom transfer. It is possible that such substances have stabilized at room temperature since no concentration increase after annealing was found for the substances eluting after anthracene in the chromatographic analysis. Two anthracene molecules cross-linked by radiation into one radical as proposed by Blum *et al.*,¹ could also react bimolecularly

with another similar radical to form one dihydroanthracene molecule and three anthracene molecules and thus could be an alternative explanation of the dihydroanthracene yield. Further information is required before either mechanism can be excluded.

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