APPENDIX

Nuclear-Magnetic-Resonance Spectrum of a Sulphone Derivative of Chlorogenoquinone

By N. F. JANES

*Department of Insecticides and Fungicides, Rothamsted Experimental Station, Harpenden, Herts.**(Received 3 December 1968)*

The nuclear-magnetic-resonance spectrum of the sulphone obtained by oxidation of chlorogenic acid in the presence of benzenesulphinic acid (Pierpoint, 1966) was recorded for a 10% (w/v) solution in dimethyl sulphoxide. The spectrum showed peaks on the τ scale relative to tetramethylsilane as internal standard: at 1.7 (*d*, 1H) and 3.8 (*d*, 1H) ($J = 16$ cyc./sec.) due to protons of $-\text{CH}=\text{CH}-$ (*trans*); at 2–2.5 (*m*, 6H) due to protons of the $\text{C}_6\text{H}_5\cdot\text{SO}_2$ group and 1 aromatic proton on the phenolic ring; at 2.8 (*s*, 1H) due to the other proton on the phenolic ring; at 4.5–8.5 τ (*m*) due to the remaining protons of the molecule and of the solvent. The spectrum is consistent with the suggested formula of the sulphone:

The singlet nature of the resonance of one proton on the phenolic ring argues against this proton being *ortho*- or *meta*- to another aromatic proton, and shows that the $\text{C}_6\text{H}_5\cdot\text{SO}_2$ group is substituted into the 6' position of the phenolic ring of chlorogenic acid.

REFERENCE

Pierpoint, W. S. (1966). *Biochem. J.* **98**, 567.