The ESR Spectrum of the Phthalonitrile Anion Radical

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(Received December 27, 1962)

Though the ESR spectra of many organic anion radicals have been investigated, that of phthalonitrile has not yet been reported on*. When phthalonitrile was reduced in dimethoxyethane (DME) with potassium or sodium, the anion radical was formed.

Thus Fig. 1's ESR hyperfine spectrum of the radical prepared with potassium agrees with the calculated value of Fig. 2, assuming that the coupling constants are $\alpha_{N_{CN}}=1.75$ gauss, $\alpha_{H_5}=\alpha_{H_4}=0.37$ gauss and $\alpha_{H_3}=\alpha_{H_6}=4.11$ gauss respectively.

On the other hand, Fig. 3's ESR spectrum of the same radical reduced with sodium appears to be different from that reduced with potassium, but one can construct a calculated spectrum similar to that of Fig. 2 provided that each line in Fig. 1 will split further into

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* The ESR spectra of the electrolytically-generated benzonitrile negative ion have been reported by P. Ludwig and R. N. Adams in *J. Chem. Phys.*, **37**, 828 (1962).

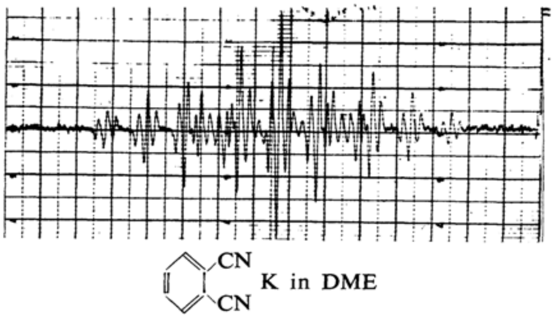

Fig. 1. ESR spectrum of phthalonitrile anion radical reduced with potassium in DME.

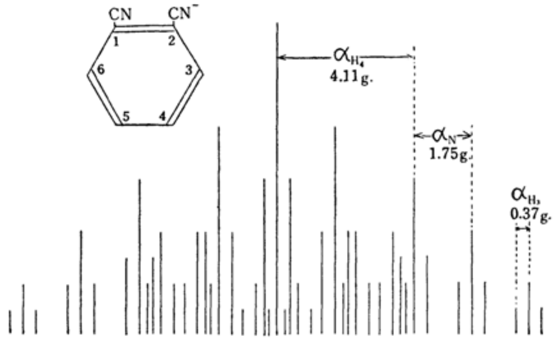

Fig. 2. Calculated spectrum of phthalonitrile anion radical.

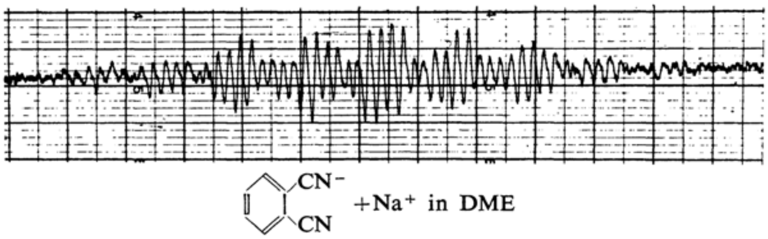

Fig. 3. ESR spectrum of phthalonitrile anion radical reduced with sodium in DME.

four, as is shown in Fig. 3, because of the hyperfine interaction of the unpaired electron spin with the sodium nuclear spin[1], whose coupling constant would be 0.23 gauss.

The ESR spectra of other aromatic nitriles will be reported on soon.

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[1] N. M. Atherton and S. I. Weissman, *J. Am. Chem. Soc.*, 83, 1330 (1961).