

Electron Spin Resonance Spectrum of BH_3^-

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WE have studied the electron spin resonance spectrum of γ -irradiated polycrystalline potassium tetrahydridoborate at 77°K . The main paramagnetic species stabilised at this temperature has been identified as the radical anion of monoborane, BH_3^- . Our identification is based on the following observations:

- (i) The radical contains one boron atom and three equivalent protons.
- (ii) The isotropic proton hyperfine coupling, although less than that for the isoelectronic

methyl radical, is nevertheless quite reasonable for BH_3^- .

- (iii) The isotropic ^{11}B hyperfine coupling is very close to expectation for BH_3^- , the corresponding U -values¹ for BH_3^- , CH_3 , and NH_3 all being close to 3.5, which indicates unit spin-density in a $2p$ -orbital on boron.

At least two other paramagnetic species are present in γ -irradiated potassium tetrahydridoborate and full details of these results will be reported later.

TABLE

Electron spin resonance parameters for XH_3 radicals
Hyperfine coupling constants (gauss)

Radical	$A_{180}(\text{X})$	$A_{180}(\text{H})$	g_{av}	U^{X} ^a	Reference
$^{11}\text{BH}_3^-$	(+) 24	(-) 16.5	2.0013	3.3	This work
$^{13}\text{CH}_3$	(+) 41	(-) 23.0	2.0026	3.7	2,3
$^{14}\text{NH}_3^+$	(+) 19.5	(-) 25.9	2.0035	3.5	4

^a $U^{\text{X}} = 100 A_{180}(\text{X})/\rho_{\text{X}} \cdot A^\circ(\text{X})$ where ρ_{X} , the spin density on X, is taken as unity and $A^\circ(\text{X})$ is the calculated hyperfine coupling for one electron in the $2s$ -orbital of X.

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