

CCA-655

539.124.143

Note

## ESR Parameters of the $\text{BF}_2$ Radical

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Received December 21, 1970

Recently Nelson and Gordy<sup>1</sup> measured ESR parameters (g-factor, a) of the  $\text{BF}_2$  radical. The authors proposed the geometry of the radical and from the analysis of the hyperfine structure deduced the spin densities on  $^{10}\text{B}$ ,  $^{11}\text{B}$  and F. In this note we point out agreement of the SCF semiempirical (INDO<sup>2</sup>) results with the results of Nelson and Gordy. INDO calculation with the geometry from ref. 1 puts the unpaired electron in the  $\sigma$  molecular orbital. The calculation of the g-factor was done using the standard approach<sup>3</sup>. Spin densities  $Q_{2s}$  were obtained by the perturbation theory<sup>4</sup> in connection with the restricted Hartree-Fock method. The expressions are of the form (notation from ref. 4):

$$q_{vw} = p_{vw}^o - \frac{1}{4} \sum_r \sum_s (\pi_{vwrs}^\alpha + \pi_{vwrs}^\beta) \sum_t \sum_u p_{tu}^o \quad (rt/us)$$

The results (Table I) show good agreement with the experiment and with the results ( $Q_{2s}$ ) deduced by Nelson and Gordy. The hybridization proposed<sup>1</sup> for the  $\text{BF}_2$  radical is qualitatively correct.

TABLE I

*g*-Factor, Spin Density  $Q_{2s}$  and Isotropic Coupling *a* (MHz) for  $\text{BF}_2$

	a	a (exp.)	$Q_{2s}$	$Q_{2s}$ (ref. 1)	g	g (exp.)
$^{10}\text{B}$	322	278	0.476	0.41		
$^{11}\text{B}$	961	826	0.476	0.41	2.0009	2.0012
F	508	532	0.010	0.011		

### REFERENCES

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**IZVLEČEK****ESR parametri  $\text{BF}_2$  radikala***M. Žaucer in A. Ažman*

Semiempirično SCF metodo smo uporabili za določitev  $g$ -faktorja in izotropne konstante  $a$  radikala  $\text{BF}_2$ . Ujemanje s eksperimentalno določenima  $g$  in  $a$  potrjuje hibridizacijo, kot sta jo predpostavila Nelson in Gordy<sup>1</sup>.

KEMIČNI INŠTITUT »BORIS KIDRIČ«

ODDELEK ZA KEMIJO

UNIVERZA V LJUBLJANI

Sprejeto 21. decembra 1970.