The Conformation of Borazole Derivatives

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IN the extension of our studies of phenyl substituted borazoles,[1] we have now examined the infrared spectra of the analogous series of *N*-triaryl- and *B*-triaryl-borazoles $(HBNAr)_3$ (I) and $(ArBNH)_3$ (II) respectively. Compounds (II) in dilute carbon tetrachloride solution are all typified by the presence of a very strong, single, sharp N–H stretching mode in the region 3433—3440 cm.$^{-1}$ We have previously suggested[2] that the presence of such an N–H stretching band indicates polarization of the N–H bond resulting from N→B p_π—p_π bonding. We can therefore suggest that (II), like the analogous *B*-triaryl-*N*-trimethylborazoles,[1] have considerable B–N double-bond character.

The ring deformation modes of *B*-triaryl-*N*-trialkylborazoles were easily identified[1] in the range 728 ± 8 cm.$^{-1}$, and the same vibrational mode is now observed in the spectra of (II) at approximately 750 cm.$^{-1}$ We failed to observe this ring deformation mode in *B*-trimethyl-*N*-triarylborazoles, and suggested[1] that this indicated that B–N π-bonding is weak.

In the present work we find that compounds (I) also do not exhibit these B–N deformations, and in addition have observed multiplicity of the B–H stretching modes, *e.g.*, in (I) (Ar = Ph) four $\nu_{\text{B-H}}$ bands are observed at 2602, 2565, 2519, and 2508 cm.$^{-1}$ The frequencies and relative intensities of these absorption bands are invariant with dilution in carbon tetrachloride. There are thus two sets of B–H stretching modes, in each case the higher frequency, and weaker, band arising from the vibration involving the ^{10}B isotope, thus:—

$$\left\{\begin{array}{ll} {}^{10}\text{B–H} & 2602 \\ {}^{11}\text{B–H} & 2565 \end{array}\right\} \text{ and } \left\{\begin{array}{ll} {}^{10}\text{B–H} & 2519 \\ {}^{11}\text{B–H} & 2508\text{ cm.}^{-1} \end{array}\right\}$$

The presence of two sets of infrared-active B–H stretching modes instead of one, as required for D_{3h} symmetry, indicates that in each case the *B*-substituents and the ring are not coplanar. Gupta and Porter,[3] in a study of solid boroxine $(HBO)_3$ (III) found two fairly intense B–H stretching modes in the infrared spectrum and therefore suggested that a similar situation occurred in solid (III).

We therefore suggest that the absence of the infrared-active B–N ring deformation mode in the 730 cm.$^{-1}$ region may be considered as being diagnostic of the non-coplanarity of the borazole ring and *B*-substituents.

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[1] J. E. Burch, W. Gerrard, M. Goldstein, E. F. Mooney, D. E. Pratt, and H. A. Willis, *Spectrochim. Acta*, 1963, **19**, 889.

[2] I. M. Butcher, W. Gerrard, E. F. Mooney, R. A. Rothenbury, and H. A. Willis, *Spectrochim Acta*, 1962, **18**, 1487.

[3] S. K. Gupta and R. F. Porter, *J. Chem. Phys.*, 1963, **67**, 1286.