

Fig. 1.—Variation of product distribution with triplet excitation energy of the sensitizer.

triplets are produced and give large amounts of cyclohexenes on reaction with isoprene. Sensitizers having less than 53 kcal. excitation energy cannot transfer energy efficiently to either isomeric form of the diene. Under such circumstances transfer probably does not involve Franck-Condon excitation of the acceptor and follows rules which we do not presently understand.

Although the terminology was somewhat different, Havinga has discussed the photoisomerization of precalciferol and related compounds in terms of stereoisomeric excited states.<sup>12</sup>

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(12) V. E. Havinga, *Chimia*, **16** (1962).

(13) Du Pont Summer Fellow, 1962.

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### THE STRUCTURE OF $C_2H_5NH_2B_8H_{11}NHC_2H_5$

Sir:

The complete geometrical structure of  $EtNH_2B_8H_{11}NH_2Et$ , including location of all H atoms attached to the boron framework, has been solved by three-dimensional X-ray diffraction study. This compound is the first derivative of a boron hydride of the hitherto uncharacterized  $B_8$  icosahedral fragment. This compound was originally thought<sup>1</sup> to be  $EtNH_3^+B_9H_{12}NH_2Et^-$ , from its preparation by reaction of ethylamine with  $B_9H_{13}SET_2$ , and its structure was therefore believed to be closely related to the known  $B_9N_{13}NCCH_3$  structure.<sup>2</sup> However, loss of  $BH_3$  has apparently occurred in this preparation, and further study may establish its fate. This new result does not exclude the possibility of at least a transient  $B_9H_{12}L^-$  anion if, for example, the electron pair donor L is pyridine.<sup>1</sup>

If one replaces one bridge H atom in the previously suggested<sup>3</sup>  $B_8H_{12}L$  structure by a bridged  $NR_2$  group ( $R = H$  or alkyl) the relation of this structure to bonding principles<sup>4</sup> of boron hydrides becomes clear. This

(1) B. M. Graybill, A. R. Pitochelli and M. F. Hawthorne, *Inorg. Chem.*, **1**, 626 (1962).

(2) F. E. Wang, P. C. Simpson and W. N. Lipscomb, *J. Chem. Phys.*, **35**, 1335 (1961).

(3) W. N. Lipscomb, *J. Inorg. Nucl. Chem.*, **11**, 1 (1959), especially the formula on p. 3.

(4) W. N. Lipscomb, *Proc. Natl. Acad. Sci. U.S.A.*, **47**, 1791 (1961) p. 1792, rule (3).

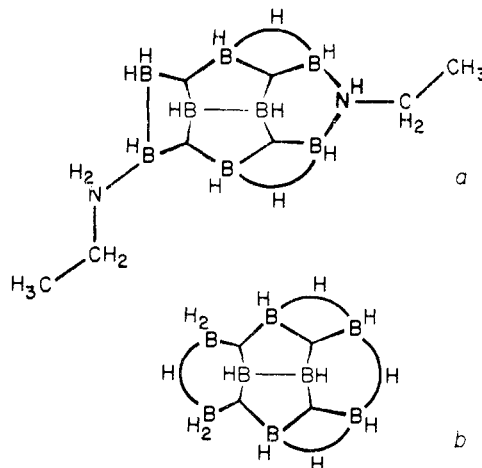


Fig. 1.—(a) The geometrical structure and a valence structure<sup>3</sup> of  $C_2H_5NH_2B_8H_{11}NHC_2H_5$ . (b) The topologically equivalent but undiscovered  $B_8H_{14}$  structure,<sup>3,6</sup> in which intramolecular tautomerism of extra BH and H bridges may occur.<sup>7</sup> The boron arrangement is an icosahedral fragment.

The bridge H between two  $BH_2$  groups in b is present in  $B_2H_6$  and  $B_4H_8^-$ , but not in known higher hydrides. If a steric problem exists here, it might be relieved by H rearrangement to 4412  $B_8H_{14}$  of symmetry  $C_2$ , by loss of bridge H<sup>+</sup> to give  $B_8H_{13}^-$ , or by loss of H<sub>2</sub> to give  $B_8H_{12}$  of symmetry  $C_2$  or  $C_2$ .

replacement is known previously<sup>5</sup> only in  $B_2H_6$ , which yields  $B_2H_5NR_2$ , and therefore  $EtNH_2B_8H_{11}NH_2Et$  is the first such example among the higher boron hydrides. The boron arrangement is that suggested by the  $B_8H_{14}$  proposal of 4412 topology<sup>6</sup> or by the closely related  $B_8H_{13}^-$  of 3422 topology,<sup>3</sup> both of which are implied by the present study as stable species or tautomers related by H atom rearrangements. It may be noted that the  $B_8H_{11}$  residue is bifunctional and hence may serve as the basis for a polymer, as do the  $B_{10}H_{12}L_2$  compounds.

The crystals are monoclinic, of symmetry  $P2_1/a$ , with four formula weights per unit cell, which has parameters  $a = 24.35$ ,  $b = 5.98$ ,  $c = 9.01 \text{ \AA}$  and  $\beta = 94^\circ 50'$ . Four molecules of  $B_8H_{24}C_2N_4$  per unit cell give a calculated density of  $0.95 \text{ g. cm.}^{-3}$  in agreement with the measured value of  $0.94 \text{ g. cm.}^{-3}$ . The formula  $C_2H_5NH_3^+B_9H_{12}NH_2C_2H_5^-$  yields a calculated density ( $1.02 \text{ g. cm.}^{-3}$ ) which is too large. At the present stage of refinement the disagreement factor,  $R = \frac{\sum ||F_0| - |F_c||}{\sum |F_0|}$ , is 0.150 for the 1566 observed X-ray diffraction maxima.

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(6) R. E. Dickerson and W. N. Lipscomb, *J. Chem. Phys.*, **27**, 212 (1957).

(7) W. N. Lipscomb, "Advances in Inorganic and Radiochemistry," Vol. I, 1959, Academic Press, Inc., New York, N. Y., p. 148.

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### THE HYDROGEN CARRIER TECHNIQUE FOR THE PYROLYSIS OF TOLUENE AND DEUTERATED TOLUENES

Sir:

The results of irradiating liquid toluene with gamma rays,<sup>1</sup> treating liquid toluene with hydrogen atoms,<sup>2</sup> and subjecting gaseous toluene to a microwave discharge<sup>3</sup> differ from the results of pyrolyzing toluene<sup>4</sup>

(1) R. B. Ingalls, *J. Phys. Chem.*, **65**, 1605 (1961).

(2) R. B. Ingalls and J. R. Hardy, *Can. J. Chem.*, **38**, 1734 (1960).