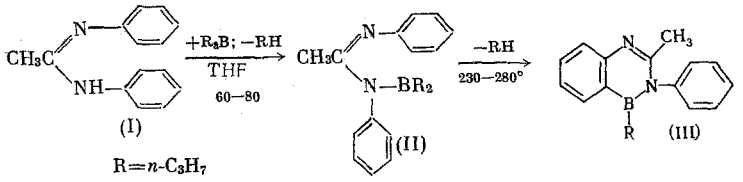
BORON-CONTAINING ANALOG OF 3,4-DIHYDROQUINAZOLINE

B. M. Mikhailov and V. A. Dorokhov

UDC 542.91:547.1'127:547.856.1

The crystalline N-di-n-propylboryl-N,N'-diphenylacetamidine (II) was obtained when a mixture of N,N-diphenylacetamidine (I) and tri-n-propylborane in THF was refluxed. Based on the data of the ^{11}B NMR spectra, this compound is associated (probably the dimer). The pyrolysis of (II) (at 230-280°C) leads to intramolecular cyclization, with the cleavage of propane (from the C_3H_7 group and the o-hydrogen of the phenylimino group) and the formation of 3-phenyl-4-n-propyl-2-methyl-3,4-dihydro-4-boraquinoazoline (III), which is a number of a new type of heterocyclic boron compounds.



A solution of 28.5 g of (I) and 23.7 g of tri-n-propylborane in 30 ml of THF was refluxed until the propane evolution ceased, after which the THF and excess tri-n-propylborane were vacuum-distilled. The residue [crude (II)] was heated at 230-280° for 5 h (3.4 liters of propane was evolved, contaminated with a small amount of propylene). Distillation gave 21.0 g [60%, when based on (I)] of (III), bp 148-153° (1 mm), mp 70-75°. ^{11}B NMR spectrum at 180°: −44 ppm (standard = $Et_2O \cdot BF_3$). NMR spectrum in CCl_4 (δ, ppm): 0.60-1.60 (C_3H_7, multiplet), 2.03 (CH_3, singlet), 6.72-8.05 ($2-C_6H_5$, multiplet). The structure of (III) was also confirmed by the elemental analysis and the mass and IR spectral data.

N. D. Zelinskii Institute of Organic Chemistry, Academy of Sciences of the USSR. Translated from Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya, No. 11, pp. 2649, November, 1973. Original article submitted July 25, 1973.