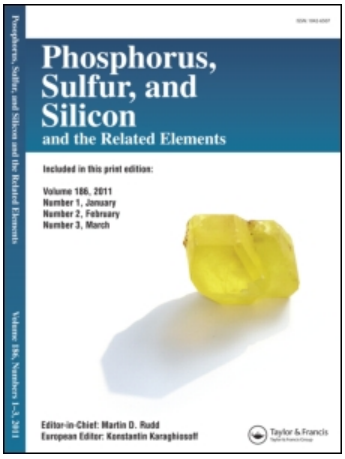

Phosphorus, Sulfur, and Silicon and the Related Elements

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Molecular Structures of 1-Dibutylboryl-2-Diphenyl-Phosphino-1-Butyl-2-Phenylethene and ITS Derivatives

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MOLECULAR STRUCTURES OF 1-DIBUTYLBORYL-2-DIPHENYL-PHOSPHINO-1-BUTYL-2-PHENYLETHENE AND ITS DERIVATIVES

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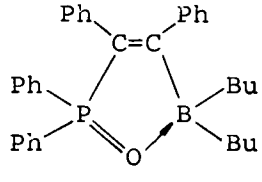
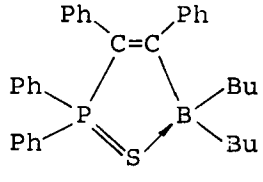
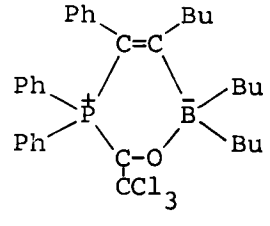
The X-ray crystal structure study of 1-dibutylboryl-2-diphenylphosphino-1-butyl-2-phenylethene (I) revealed that this molecule has Z-conformation respective to C=C bond. The P-B distance is 2.104(5) Å and the P-C=C and B-C=C bond angles are decreased to 96.1(3) and 109.3(4)°. This is the evidence of P → B dative interaction. The ab initio calculations of the model borylphosphinoethene H_2P-CH=CH-BH_2 with full geometry optimization showed that the phosphorus lone electron pair is shifted towards boron by 0.26 Å. Thus the existence of the dative P → B bond is confirmed. The reaction of inserting oxygen, sulfur or trichloroacetic acid anhydride into P → B bond of (I) leads to the formation of 5- and 6-membered ring compounds.



II



III



IV

Molecules II and II have planar rings and the 6-membered ring of IV adopts the sofa conformation. The P=E (E=O, S) bond in molecules II and III is lengthened by 0.05 Å compared with triphenylphosphine oxide and sulfide due to the E → B bond formation.