# The Use of Quantum-Chemical Semiempirical Methods to Calculate the Lattice Energies of Organic Molecular Crystals. Part III: The Lattice Energy of Borazine ($B_3N_3H_6$) and its Packing in the Solid State*

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*Dedicated to Professor Syd Hall, PhD, on the occasion of his 65th birthday*

A previously presented quantum-chemical scheme has been used to calculate the lattice energies of borazine ($B_3N_3H_6$), the low pressure polymorph of benzene ($C_6H_6$), and of borazine in the low-pressure benzene lattice utilizing some frequently used semiempirical methods (CNDO/2, INDO, MINDO/3, MNDO, AM1, PM3, MSINDO). With all methods the lattice energy of the title compound was found to be less favourable than that of isoelectronic benzene, which offers an explanation of the significantly lower melting point of $B_3N_3H_6$. Calculation of the lattice energy of borazine in the crystal lattice of the low-pressure modification of benzene revealed that the interactions between the molecules in this environment are not so stabilizing as those in its own lattice. This is predominantly due to a less favourable contribution of the dispersion energy. The semiempirical results have qualitatively been confirmed by quantum-chemical calculations on small molecular clusters at the MP2/6-31+G*//HF/6-31+G* level of *ab initio* theory. In these calculations we assumed pairwise additivity of the intermolecular interactions and calculated the energy of interaction between a reference molecule and all those neighbours to which the shortest intermolecular distance does not exceed 3 Å.

*Key words:* Borazine; Lattice Energy; Calculations; Semiempirical Methods.