

**s9.m2.p5** Quantum Chemical Calculations on the Crystal Structure of Borazine ( $B_3N_3H_6$ ).

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The lattice energies of borazine [1] ( $B_3N_3H_6$ ) and the low pressure polymorph of benzene ( $C_6H_6$ ) have been calculated using a recently developed semiempirical quantum chemical method. Within the framework of this method the lattice energy is calculated as the sum of the dispersion-, the induction-, the repulsion, and the electrostatic energy [2-5]. The semiempirical results have been confirmed by *ab initio* calculations at the MP2/6-31+G\*/HF/6-31+G\* level [6,7]. In these non-empirical calculations we assumed pairwise additivity and calculated the energy of interaction between a reference molecule and all those neighbours in the crystal lattice to which the shortest intermolecular distance does not exceed  $3\text{Å}$ .

The lattice energy of borazine was found to be significantly less favourable than that of the low pressure polymorph of isoelectronic benzene. While this result offers an explanation for the lower melting point of the title compound, it does not provide an answer to the question why the packing of the  $B_3N_3H_6$  molecules in the solid state is significantly different from that of benzene. However, 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 clearly less stabilizing than those in its own lattice.

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