Molecular Structure of Bis(trimethylsilyl) Hypophosphite $HP(OSiMe_3)_2$ by Gas-Phase Electron Diffraction and Quantum Chemistry

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Abstract — Geometric parameters and conformation of the bis(trimethylsilyl)hypophosphite molecule were determined by gas-phase electron diffraction and quantum-chemical calculations. The molecule has an asymmetric structure, including an asymmetric $P(OSiMe_3)_2$ group. The principal geometric parameters are as follows: (r_a; in parentheses are standard deviations): bond lengths: P–O 1.616 and 1.633(1), Si–O 1.670(1), Si–C 1.892(1), C–H 1.097(3) Å; bond angles: OPO 100.8(8), POSi 133.3, and 138.4(3)°; torsion angles about P–O bonds 120(2) and 41.(3)°; and torsion angles about Si–O bonds are 145 and –178(4)°.