

## Diagrams of isoshielding lines of C-N bonds and nitrogen and phosphorus lone pairs

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### Abstract

Diagrams of isoshielding lines in the vicinity of lone pairs of nitrogen and phosphorus atoms, as well as a C-N bond, have been calculated. The magnetic shielding constants of the protons were calculated by the gauge-invariant atomic-orbital method with the use of localized molecular orbitals and expansions of the atomic wave functions in Gaussian functions. The diagrams of the isoshielding lines have been used for the evaluation of chemical shifts in piperidine derivatives for the purpose of accounting for the experimentally observed tendencies in chemical shifts. © 1986 Plenum Publishing Corporation.

<http://dx.doi.org/10.1007/BF01004515>

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