

## Contributions of localized MO's to the magnetic shielding constants of protons in YPX3 molecules

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### Abstract

1. Calculations of the magnetic shielding constants of the protons in the  $O=PMe_3$  and  $S=PMe_3$  molecules have been carried out. 2. The decisive contribution to the shielding of a proton is made by the C-H bond itself, and it is transferred fairly completely from one molecule to another. 3. Diagrams of the isoshielding lines of the P-O and P-C bonds have been calculated, and they can be used for the analysis of the chemical shifts caused by the influence of these bonds in systems with similar environments for the phosphorus atom. © 1986 Plenum Publishing Corporation.

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