

## individual gauge for localized orbitals (IGLO)

A method of calculation of nuclear shieldings, in which localized molecular orbitals associated with inner shell, bonding orbitals, and lone pairs have unique origins for the calculation of diamagnetic and paramagnetic terms. With this method, satisfactory estimates of NMR chemical shifts for elements in the first and second rows can be achieved in *ab initio* calculations with basis sets of moderate size provided sufficiently accurate molecular geometries are used.

**Source:**

PAC, 1999, 71, 1919 (*Glossary of terms used in theoretical organic chemistry*) on page 1946