A tight-binding treatment for calculations of NMR chemical shifts

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The wave function calculated with the Density-functional based tight-binding (DFTB) method is used as a basis for calculations of nuclear magnetic shieldingsin molecules. As an illustrative example for the application of this method, results for ^{13}C NMR chemical shifts in fullerenes - from C_{60} to C_{84} - are shown. The magnetic shieldings are computed with the sum-over-states (SOS) individual gauge local orbitals (IGLO) method. Qualitative agreement with experimental patterns, determination between alternative isomeric possibilities and a correlation between local geometry and calculated shift are reported.