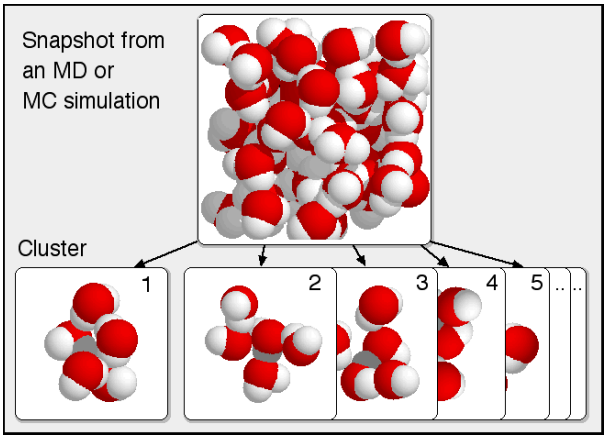

Figure 11.1 In the cluster method one (as in the figure) or more snapshots from a simulation are used to extract clusters around atoms of interest. Here clusters of size five are selected around water protons of interest (dark proton in the center of the clusters) to calculate the proton chemical shielding. Each cluster is treated as a supermolecule in a quantum chemical calculation and the average is obtained to yield the chemical shielding in the liquid.

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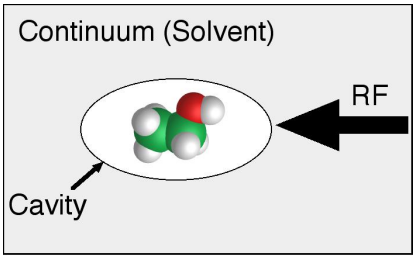

Figure 11.2 The continuum or reaction field methods place the solute molecule in a cavity and treat the solvent as a continuum, which reacts on the molecular electric field by a reaction field (RF). The cavity might be a sphere, an ellipsoid as shown in the figure, or a more complicated shape following the surface of the molecule. One of the problems of these methods for the calculation of NMR properties seems to be the extreme sensitivity of the latter to the (empirical) size of the cavity.

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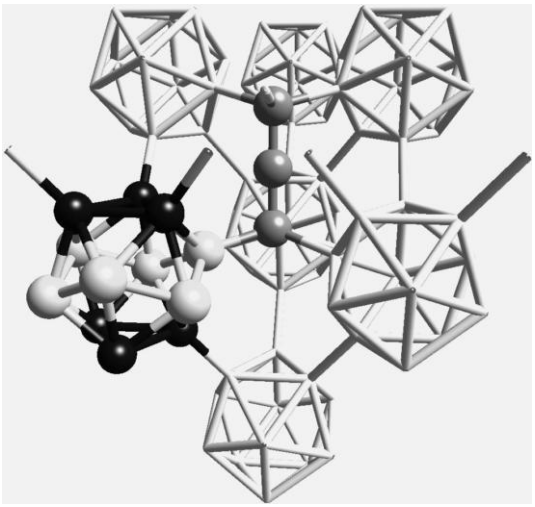

Figure 16.2 Atomic structure of B_4C. The black atoms are on the so-called *polar* sites, bonded to neighboring icosahedra. The white atoms form a puckered hexagon and are in *equatorial* sites. The gray atoms form the *chain*, to which the *equatorial* atoms are bonded.

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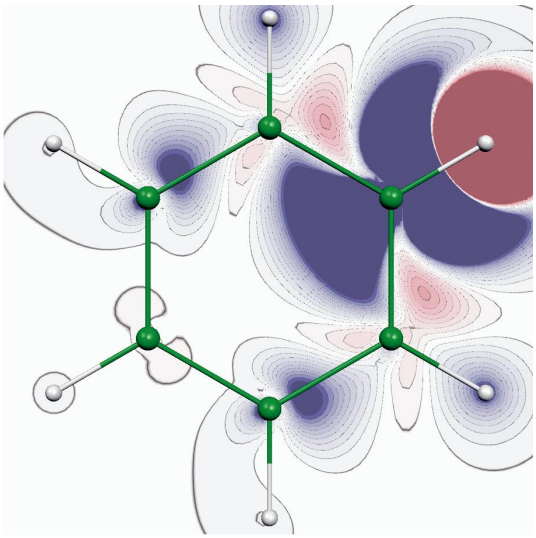

Figure 19.1 Visualization of the spin density in benzene obtained from single FPT with the center of perturbation on the hydrogen at the right upper part of the plot.

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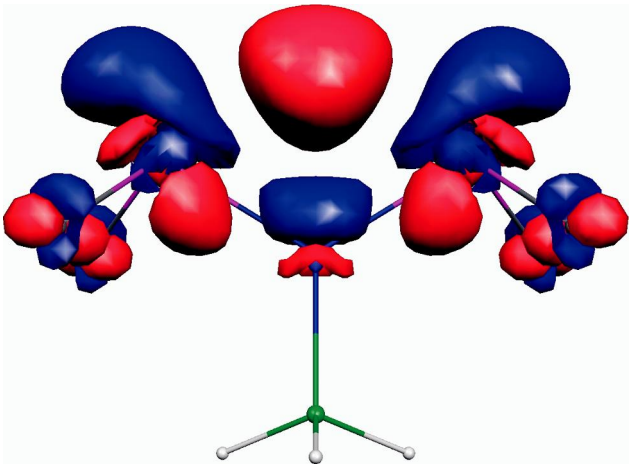

Figure 19.2 Visualization of ^2J(P–P) coupling energy density (CED) in bis(diflurophosphino)methylamine.

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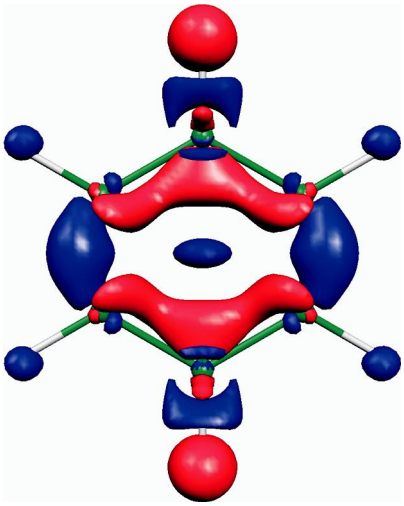

Figure 19.3 Visualization of ^{5}J(H–H) coupling electron deformation density (CDD) in benzene.

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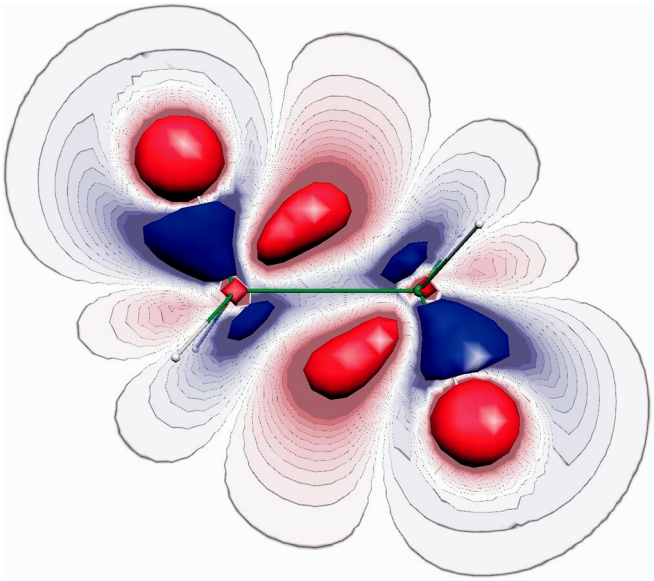

Figure 19.4 Visualization of *trans* ^3J(H–H) coupling electron deformation density (CDD) in ethane.

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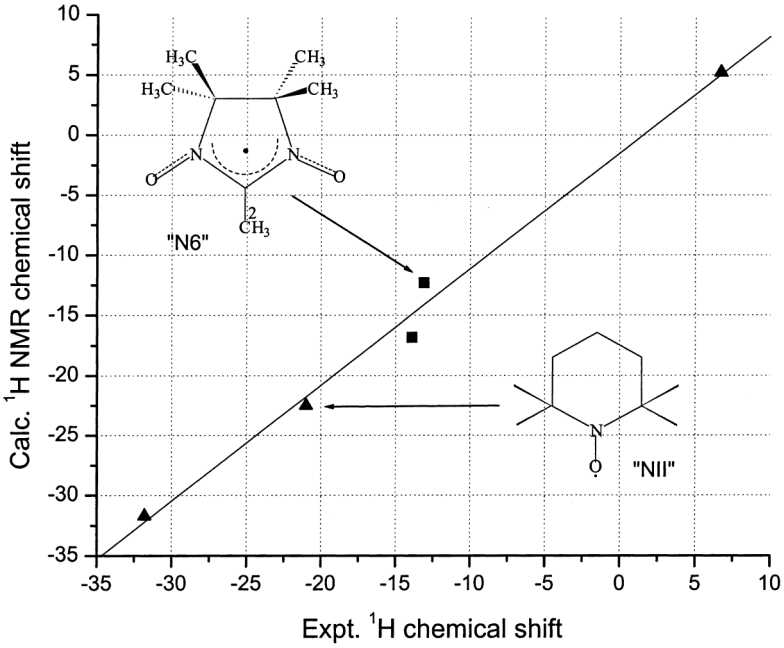

Figure 20.2 Correlation between the experimental and calculated paramagnetic NMR chemical shifts for ^{1}H nuclei in substituted nitroxide radicals. See Fig. 20.1 for details. Chemical shift of 2-CH_3 in "N6" is not shown (see text).

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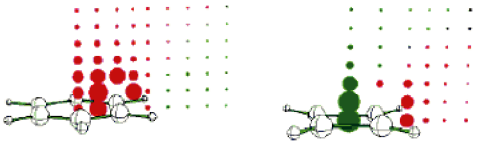

Figure 24.1 NICS grid of benzene and cyclobutadiene. The red and green colors denote negative and positive NICS values, respectively.

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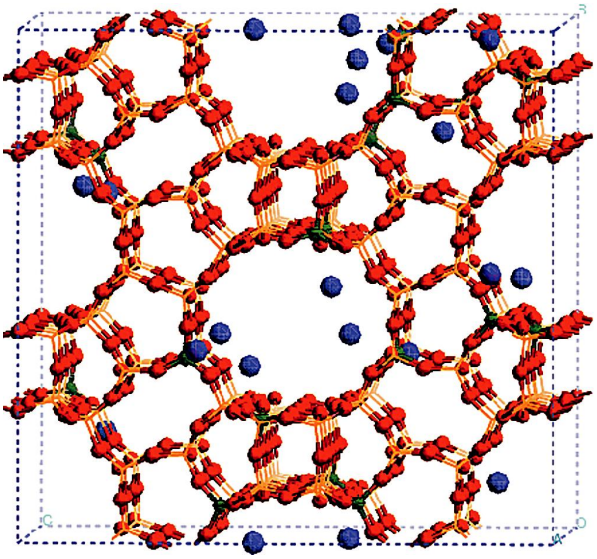

Figure 28.1 Zeolite b (4 unit cells) with Si/Al = 13; yellow sticks represent Si, green balls Al, red balls O, blue balls Na^+.

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