Relativistic four-component study of through–space spin–spin coupling constants

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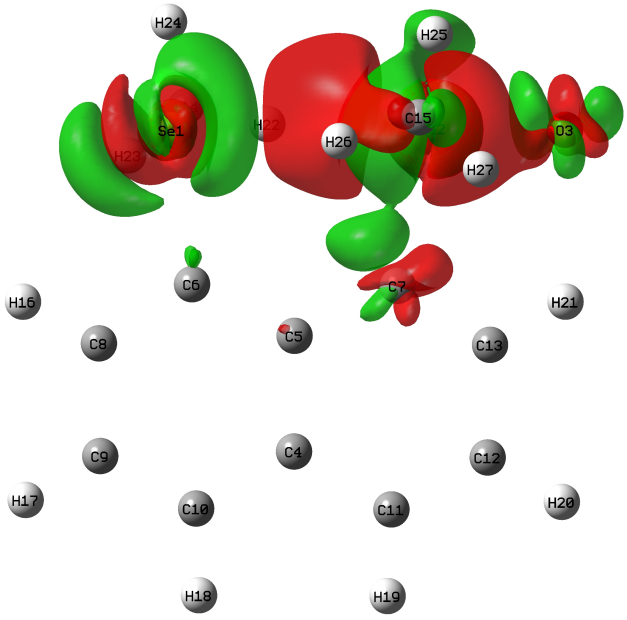
Four-component approach at the density functional level of theory is used to study and visualize through-space NMR spin-spin coupling constants (SSCC). The values of SSCCs of the type Se-Se, Se-Te and Te-Te in three similar molecules determined in the relativistic and nonrelativistic approach are compared. We discuss the first-order current densities induced by the nuclear magnetic dipoles, and different possibilities to visualize the relativistic effects are considered.



Se-Se coupling in peri-substituted naphthalene, $\vec{j}^{Se2,z} \cdot \vec{A}^{Se1,z}$.

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References

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