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Nota di contenuto	Contents; Preface to the ESPA-2014 special issue; AMOEBA force field parameterization of the azabenzenes; 1 Introduction; 2 Computational details; 2.1 Quantum calculations; 2.2 Force field; 2.2.1 The AMOEBA formalism; 2.2.2 Details of AMOEBA calculations; 2.3 Parameterization; 2.4 Atomic multipoles; 3 Force field validation and refinement of vdW parameters; 3.1 Bonded interactions, force constants, and vibrational frequencies; 3.2 Molecular multipoles and electrostatic potential; 3.3 Intermolecular interactions; 4 Conclusions; 5 Supporting information; References Triplet-singlet gap in structurally flexible organic diradicals1 Introduction; 2 Model systems; 2.1 Computational approach; 3 Results and discussion; 3.1 Local minima, isomers and enantiomers; 3.2 Triplet-singlet gaps; 4 Conclusions; References; Separating nuclear spin isomers using a pump-dump laser scheme; 1 Introduction; 2 Methods; 3 Results and discussion; 3.1 Pump process; 3.2 Dump

process; 4 Conclusion; References; Spin delocalization in hydrogen chains described with the spin-partitioned total position-spread tensor; 1 Introduction; 2 General formalism: spin partition of TPS tensor

3 Computational details4 Results and discussions; 4.1 Equally spaced hydrogen chains; 4.2 Dimerized chains; 4.2.1 Fixed-bond dimerized hydrogen chains; 4.2.2 Homothetic dimerized hydrogen chains; 4.3 Asymptotic behavior of the longitudinal position-spread tensors; 5 Conclusions; References; Invariant time-dependent exchange perturbation theory and its application to the particles collision problem; 1 Introduction; 2 Exchange perturbation theory (EPT), time-dependent perturbation; 3 Perturbation theory to the first order; 4 Perturbation theory to the second and higher orders

5 S-scattering and T-matrix elements6 Collisions with exchange of electrons; 7 Scattering of proton by lithium atom with electron exchange; 8 Conclusions; Appendix 1; Appendix 2; Appendix 3; References; On the definition of molecular dynamic magnetizability; 1 Introduction; 2 Electromagnetic multipole moment operators and the interaction Hamiltonian; 3 Induced electric dipole moment; 4 Induced magnetic dipole moment; 5 Change of response properties and equivalence conditions in a translation of coordinates; 5.1 Magnitude of origin-shift vectors

5.2 Translation of frequency-dependent response tensors6 Variation of frequency-dependent moments in a coordinate translation; 7 Orders of magnitude; 8 Concluding remarks; References; Toward (car)borane-based molecular magnets; 1 Introduction; 1.1 The theoretical models; 1.1.1 Two magnetic sites system; 1.1.2 Three magnetic sites systems; 1.1.3 Four magnetic sites system; 2 Results and discussion; 3 Concluding remarks; References; Theoretical analysis of vibrational modes in uranyl aquo chloro complexes; 1 Introduction; 2 Computational aspects; 3 Results and discussion; 4 Conclusions

References

## Sommario/riassunto

This volume collects research findings presented at the 9th Edition of the Electronic Structure: Principles and Applications (ESPA-2014) International Conference, held in Badajoz, Spain, on July 2–4, 2014. The contributions cover research work on theory, methods and foundations, materials science, structure and chemical reactivity as well as environmental effects and modelling. Originally published in the journal Theoretical Chemistry Accounts, these outstanding papers are now available in a hardcover print format, as well as a special electronic edition. This volume provides valuable content for all researchers in theoretical chemistry, and will especially benefit those research groups and libraries with limited access to the journal.