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Effective Nuclear Charges for the First- through Third-Row Transition Metal Elements in Spin–Orbit Calculations

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Abstract

The effective nuclear charges (Z_{eff}), which are empirical parameters in an approximate spin–orbit Hamiltonian, are determined for the first- through third-row transition metal elements by using experimental results for the fine structure splittings in atomic terms. All calculations use multiconfiguration self-consistent-field (MCSCF) wave functions, whose active space includes nd and $(n + 1)sp$ orbitals (n is the principal quantum number), with the effective core potential (ECP) basis sets proposed by Stevens et al., augmented by one set of polarization f functions. First-order or second-order configuration interaction (FOCI or SOCI) calculations were also performed in order to understand disagreements between the MCSCF results and the experimental ones.

Disciplines

Chemistry

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