Exploring the importance of including CI wave functions in the target \( n \) expansion and in the \((n+1)\)-electron quadratically integrable function expansion

I. Fe-peaks Co IV (Cr-like): \( Z=24 : 3p^6(3d)\)

The accuracy of a series of models for the target term has been investigated including all of the 136 LS-coupled states, arising from the three manifolds \( 3s^2, 3p^4, 3d^4 \) in the R-matrix expansion.

II. Reference configurations

Mg

1. Reference configurations: \( 2s^2(2s)^2(2p)^6(3s) \) single and double excitations from the valence electrons to account for the excitation-effect calculation.
2. Reference configurations: \( 2p\alpha^2(1s)^2(2s)^2(2p)^6(3s) \) and \( 2p\beta^2(1s)^2(2s)^2(2p)^6(3p) \) allowing one 2p electron and one valence electron excitation.
3. Reference configurations: \( 2s^2(2s)^2(2p)^6(3s) \) and \( 2p\alpha^2(1s)^2(2s)^2(2p)^6(3p) \) allowing two 2p electrons and one valence electron excitation.

II. Mg-like S: \( 2p^3d^2(3s)\)

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C. Reference configurations: \( 2s^2(2s)^2(2p)^6(3s) \) and \( 2p\alpha^2(1s)^2(2s)^2(2p)^6(3p) \) allowing two 2p electrons and one valence electron excitation.

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