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**An Examination of the Configuration Averaged Hartree-Fock Procedure  
for Model Ferredoxin and Its Electronic Spectroscopy**

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**Abstract**

A configuration averaged Hartree-Fock (CAHF) procedure has been applied to a model ferredoxin  $[\text{Fe}_2\text{S}_2(\text{SH})_4]^{2-}$ . The anti-ferromagnetism and spectroscopy have been studied within the restricted open-shell Hartree-Fock (ROHF) approximation and the resulting wavefunction refined by a subsequent configuration interaction (CI). The results obtained suggest that a simple CAHF model, with spin projection, is accurate, typically producing states of the correct nature when compared with those derived from far more computer intensive ROHF-CI calculations. A general procedure is proposed which allows for the calculation of the electronic spectra of either the high spin or the anti-ferromagnetic ground states using a CI for the highest multiplicity states only. The procedure we demonstrate here can be extended to more sophisticated models of ferredoxins; i.e., systems containing more metal atoms and therefore more complex multiplicity problems.

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