

# Importance of Correlation and Scalar Relativistic effects



TM Multiplet Splitting		HF	CCSD	CCSD(T)	$\Delta$ CCSD(T)	CCSDT-3	Experiment
Fe	$^5F(d^6s^2) - ^5D(d^7s^1)$	2.106	1.103	0.993	0.975	0.954	0.87
Co	$^4F(d^7s^2) - ^4F(d^8s^1)$	1.864	0.680	0.532	0.505	0.479	0.42
Ni	$^3F(d^8s^2) - ^3D(d^9s^1)$	1.201	-0.044	-0.168	-0.210	-0.135	-0.03
	$^3F(d^8s^2) - ^1S(d^{10})$	5.694	2.180	1.658	1.487	1.299	1.71
Cu	$^2D(d^9s^2) - ^2S(d^{10}s^1)$	0.153	-1.208	-1.383	-1.434	-1.459	-1.49