Magnetic Exchange Couplings in Heterodinuclear Transition Metal Complexes based on Differential Local Spin Rotations[1] RAJENDRA JOSHI, Department of Physics and Science of Advanced Materials, Central Michigan University, Mount Pleasant, MI, 48859, USA, JORDAN PHILLIPS, Science of Advanced Materials, Central Michigan University, Mount Pleasant, MI, 48859, USA, JUAN PERALTA, Department of Physics and Science of Advanced Materials, Central Michigan University, Mount Pleasant, MI, 48859, USA — We assess the performance of a new method based on a generalized perturbative approach, which uses differential local spin rotations for the calculation of magnetic exchange couplings for the case of heterodinuclear transition metal complexes of Cu, Ni, and V. These types of complexes pose a challenge for estimating exchange couplings, mainly due to the asymmetrical spin on the metal centers and the different mapping schemes that can be applied to such systems. The reliability of calculated couplings has been examined by comparing with couplings obtained from the broken symmetry (BS) energy differences method with different exchange correlational functionals, and experimental values. Results show that our method to calculate magnetic exchange couplings can be reliably employed with heterodinuclear complexes, and gives results similar to BS energy differences, when a proper mapping is used.

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