RELATIVISTIC EFFECTS IN LIGHT MOLECULAR SYSYTEMS

G. TARCZAY, *Department of General and Inorganic Chemistry, Eötvös University, P.O. Box 32, H-1518 Budapest 112, HUNGARY*; A. G. CSÁSZÁR, *Department of Theoretical Chemistry, Eötvös University, P.O. Box 32, H-1518 Budapest 112, HUNGARY*; W. KLOPPER, *Theoretical Chemistry Group, Debye Institute, Utrecht University, Padualaan 14, NL-3584 CH Utrecht, The Netherlands*.

Relativistic energy corrections to the electronic energy have been determined for prototypical molecular systems containing light atoms [e.g. NH_3, H_2O, HNCO, $(HF)_2$]. The calculations performed at the HF and CCSD(T) levels of theory utilized first-order perturbation theory as applied to the mass-velocity (MV) and one- (D1) and two-electron Darwin (D2) terms. Both MV and D1 are substantial, but they have oposite sign, canceling out most of their effect. The D1 term has been computed for the individual atoms of the molecules. As expected, D1 for a given atom, changes little from molecule to molecule. Although D2 is small, its magnitude is comperable to the electron correlation contribution to the relativistic energy corrections. Influence of the relativistic correction on force constants, inversion barriers, and interaction energies has also been investigated.