TRANSFERRING POLARIZABILITIES FROM DIATOMICS TO LARGER MOLECULES

STEPHEN L COY, TIMOTHY J BARNUM, ROBERT W FIELD, *Department of Chemistry, MIT, Cambridge, MA, USA*; BRYAN M. WONG, *Department of Chemistry, University of California, Riverside, Riverside, Ca, USA*.

Because of the involvement of low-lying 3d levels in bonding and polarizability, calcium resembles an early transition metal. In a biological context, calcium has bonding flexibility, high availability, and is an essential component of many proteins. It is metered or gated by voltage or ligands through calcium channels, and is processed and remodeled in bone and shell structure.

In the case of diatomics, ab-initio calculations and the interpretation of Rydberg spectra can be used to infer effective atomic charges, and dipole-dipole or dipole-quadrupole polarizability for the Ca cation, and charge and dipole-dipole polarizability for the ligand. Calculations with an external point-charge perturbation can provide additional types of molecular polarizability values.

Calculations on calcium difluoride, CaF2, which, surprisingly, is non-linear, can provide the same type of information about the atomic constituents. We compare the metal and ligand effective atomic electric properties of the diatomic and triatomic, and compare to the values used for biological systems.