

MOLECULAR QUADRUPOLE MOMENTS AND ELECTRONIC STRUCTURE

JAMES F. HARRISON, *Department of Chemistry and Center for Fundamental Materials Research, Michigan State University, East Lansing MI 48824-1322*; DANIEL B. LAWSON, *Department of Chemistry, Calvin College, Grand Rapids MI.*

Molecular quadrupole moments are notoriously difficult to interpret for several reasons, one of which is that they have a nuclear and an electronic contribution, which have similar magnitudes and opposite signs. While the same situation exists for dipole moments we seem to have no trouble in relating these to the molecular charge distribution. The reasons for this ease of conceptualization for dipole moments will be identified and the same strategy will be used to interpret the quadrupole moments of the homonuclear diatomics, H₂ through Cl₂.