Heme electronic structure calculations with band parameters from optical absorption spectra ARTHUR BRILL, Professor of Physics Emeritus University of Virginia, MARK CARLSON, Science Faculty, Illinois Mathematics & Science Academy — Central energies, bandwidths, peak absorptivities, oscillator strengths and transition dipole matrix elements are available from bandanalysis of optical absorption spectra for the visible and near UV regions of the aquo, fluoride, azide and cyanide complexes of horse metmyoglobin (M. L. Carlson and A. S. Brill, paper in preparation). The circular orbit model of porphin structure is applicable to related structures such as heme, and is useful for identifying $\pi - \pi$ transitions responsible for the B bands in the Soret and the Q bands in the visible. The other transitions from this bandanalysis are identified as visible n-$\pi$ (four for the aquo complex, five for both the F$^-$ and CN$^-$ complexes, six for the NH$_3^-$ complex) and near ultraviolet beyond the Soret (seven for the aquo, fluoride and cyanide complexes, six for the azide). With the circular orbit model, average inner and outer radii of the structure of the heme chromophore are calculable from the lower and higher pairs of band center energies of $\pi - \pi$ transitions. These radial distances are in approximate agreement with structural data from x-ray diffraction.