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Using the IDE to Assemble a Z80 Program:. 2 Â» 1 DAT AVLZ A26 JNZ 7157 Â» 1 DAT. "0Â« 15 15 15 15 Â« 15 15 15 15 Â« 15 Â« 15 15 Â« 15 15 15 15.Electronic structure and bonding of the ground and intermediate states of the reactants and transition states of phenyl hydroxylation by peroxyhemoglobin. The absorption spectrum of hemoglobin provides the convenient means to determine its electronic structure in the vicinity of the ligand heme. Spectral shifts in the Soret band reveal the ligand-induced perturbations of the iron ion's electronic structure. Two peaks are seen in the absorption spectrum; the low-energy (L) peak corresponds to the transition between the electronic ground state and the lowest eigenstate of the iron ion, the intermediate state (I), the highest energy (H) peak corresponds to the transition between the intermediate state and the dissociative state. The bending of the spectrum is a result of the reduction in the Fe-O-Fe angle which occurs in the transition to the dissociative state. The bending, shape, and intensity of the ligand peaks depend on whether the ligand is oxygen or a photolytic hydroxide. The ground state of the reactant (oxyhemoglobin) has the lowest energy in the heme pocket and its electronic structure is the least perturbed by the ligand. The bending of the absorption spectrum and the shift of the peak maximum toward shorter wavelength is much greater with photolytic hydroxide than with oxygen. This indicates that the most important changes in the electronic structure of the intermediate state occur upon formation of the heme pocket. This occurs because the ligand is fully electronic in the intermediate state and the distribution of electronic charge is greatest in this state. Finally, the absorption spectrum of Hb.O2 has a maximum at 545 nm, which shifts to 521 nm upon photolytic hydroxide addition; this shift is characteristic of a high-spin heme iron. The iron ion in the intermediate state has increased electronic charge, but this charge is not distributed homogeneously, because the iron ion's sixth ligand, oxygen, is in a partially ionized state. The ratio of the absorption coefficients of the H and L bands changes with the photolysis reaction; a shift to higher energy of the spectrum indicates that the iron ion is

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