116. The two limiting wavefunctions of the ground state of H_2^+ molecular ion, as the internuclear separation R goes to (i) ∞ (infinity) and (ii) 0 (zero) are ($1s_a$, $1s_b$ are 1s-orbital wave functions of hydrogen atoms *a* and *b* in H_2^+, and $1s_{He}$ is the wave function of the 1s orbital of He^+)

(a) (i) $1s_a(r)$; (ii) $1s_b(r)$ (b) (i) $1s_b(r)$; (ii) $1s_a(r)$

(c) (i) $1s_a(r_1)1s_b(r_2)$; (ii) $1s_{He}(r_1)1s_{He}(r_2)$ (d) (i) $1s_a(r)+1s_b(r)$; (ii) $1s_{He}(r)$

117. For a certain magnetic field strength, a free proton spin transition occurs at 700 MHz. Keeping the magnetic field strength constant the ^{14}N nucleus will resonate at $\left(g(p) \simeq 5.6 \text{ and } g(^{14}N) \simeq 0.4\right)$

(a) 700 MHz (b) 400 MHz (c) 200 MHz (d) 50 MHz

118. The first electronic absorption band maximum of a polar and relatively rigid aromatic molecule appears at 310 nm but its fluorescence maximum in acetonitrile solution appears with a large Stokes shift at 450 nm. The most likely reason for the Stokes shift is

(a) large change in molecular geometry in the excited state
(b) increase in dipole moment of the molecule in the excited state
(c) decrease in polarizability of the molecule in the excited state
(d) lowered interaction of the excited molecule with polar solvent

119. The un-normalized radial wave function of a certain hydrogen atom eigenstate is $(6r - r^2)\exp(-r/3)$. A possible angular part of the eigenstate is

(a) $5\cos^3\theta - 3\cos\theta$ (b) $3\cos^2\theta - 1$ (c) $\cos\theta$ (d) 1

120. Given a trial wave function $\psi_t = C_1\phi_1 + C_2\phi_2$, and the Hamiltonian matrix elements, $\int \phi_1^* H \phi_1 dv = 0$, $\int \phi_1^* H \phi_2 dv = 2.5$, $\int \phi_2^* H \phi_2 dv = 12.0$, the variationally determined ground state energy is

(a) –0.52 (b) –0.50 (c) 12.50 (d) 12.52