

Q56 Select the item that is the contribution to the energy of the $2^2S_{1/2}$ state due to $\delta\hat{H}_{\text{spin-orbit}}$.

Q57 Select the item that is the contribution to the energy of the $2^2S_{1/2}$ state due to $\delta\hat{H}_{\text{rel}}$. **H**

Q58 Select the item that is the contribution to the energy of the $2^2S_{1/2}$ state due to $\delta\hat{H}_{\text{Darwin}}$. **B**

Q59 Select the item that is the contribution to the energy of the $2^2P_{3/2}$ state due to $\delta\hat{H}_{\text{rel}}$. **E**

Q60 Select the item that is the contribution to the energy of the $2^2P_{3/2}$ state due to $\delta\hat{H}_{\text{Darwin}}$. **D**

KEY for Q56 to Q60

A 0	E $-\frac{7}{192}\alpha^2 E_R$
B $\frac{1}{48}\alpha^2 E_R$	F $-\frac{1}{24}\alpha^2 E_R$
C $\frac{1}{8}\alpha^2 E_R$	G $-\frac{5}{64}\alpha^2 E_R$
D $-\frac{1}{64}\alpha^2 E_R$	H $-\frac{13}{64}\alpha^2 E_R$

Q61 The key to Q61 contains a number of statements principally concerning the variational treatment of the hydrogen molecule ion, H_2^+ . Options in the key refer to the trial wave function

$$\psi_1 = A\psi_1(\mathbf{r}) + B\psi_2(\mathbf{r})$$

where $\psi_1(\mathbf{r})$ and $\psi_2(\mathbf{r})$ are certain given functions, and the expectation value, $\langle E \rangle$, of the total energy of the electron in the state represented by ψ_1 . The symbol R in the key is the interproton separation. Choose the *two* true statements.

KEY for Q61

- A For given R , the variational method applied to ψ_1 determines values of A and B such that $\langle E \rangle$ gives the lowest value of the total energy of the ion for that value of R that can be found with given functions $\psi_1(\mathbf{r})$ and $\psi_2(\mathbf{r})$.
- B For given R , the variational method applied to ψ_1 determines A and B such that $\langle E \rangle$ gives the lowest possible value of the electronic energy that can be found with the functions $\psi_1(\mathbf{r})$ and $\psi_2(\mathbf{r})$.
- C For given R , the variational method applied to ψ_1 finds values of A and B such that $\langle E \rangle$ gives the lowest possible value for the electronic energy for that fixed value of R .
- D In order to find the total energy of H_2^+ , the variational method must be complemented with a knowledge of how the interproton repulsion energy depends on R .
- E For given R , the variational method applied to ψ_1 gives values of A and B such that $\langle E \rangle$ gives the lowest possible value of the total energy of H_2^+ for that fixed value of R .
- F The variational method applied to ψ_1 finds values of A and B such that $\langle E \rangle$ gives the lowest

possible value for the total energy of H_2^+ .

G There is only one true statement in A-F.

Q62 and Q63 share the same key and refer to the hydrogen molecule ion, H_2^+ , discussed in Part B of Unit 16. The dissociation energy of the ion for separation into a neutral hydrogen atom in its ground state and a free proton is 2.79 eV.

Q62 What is the minimum energy required to separate the ion into two free protons and a free electron?

Q63 What is the minimum energy required to separate the ion into a free proton and a hydrogen atom in its first excited state?

KEY for Q62 and Q63

A 2.79 eV	E 13.00 eV
B 7.42 eV	F 13.61 eV
C 10.21 eV	G 16.40 eV
D 10.81 eV	H 27.22 eV

Q64 and Q65 share the same key and concern the minimum energies required to dissociate the ground state of a hydrogen molecule into various final states. In each case, you are to select from the key the item that is closest to the energy in question.

Q64 What is the minimum energy required to obtain two free protons and two free electrons?

Q65 What is the minimum energy required to obtain two hydrogen atoms?

KEY for Q64 and Q65

A 31.7 eV	E 14.7 eV
B 27.2 eV	F 13.6 eV
C 18.1 eV	G 4.5 eV
D 15.3 eV	H 2.8 eV