

Question 1

Correct

Mark 1.00 out of 1.00

Flag question

All eigenvalues of an Hermitian operator are always real numbers [1 mark]

Select one:

- True ✓
- False

The correct answer is 'True'.

Question 2

Incorrect

Mark 0.00 out of 6.00

Flag question

Harmonic Oscillator and Rigid Rotor: For the $^{12}\text{C}^{16}\text{O}$ molecule we get an absorption feature in the infra-red region at 668 cm^{-1} . In the microwave region we get a series of equally spaced lines separated by $6.6 \times 10^{11}\text{ Hz}$. Determine the potential energy of the bond when stretched to 2.1 times its equilibrium length? The answer should be in eV, correct upto three decimal places. [6 marks]

Useful Information (must use these values, if required):

$$h = 6.6 \times 10^{-34}\text{ J s}, \pi = 3.14, m_p = 1.67 \times 10^{-27}\text{ kg}$$

$$e = 1.6 \times 10^{-19}\text{ C}, c = 3 \times 10^8\text{ m s}^{-1}$$

Answer: ✗

The correct answer is: 1.519

Question 3

Correct

Mark 1.00 out of 1.00

Flag question

The one-dimensional harmonic oscillator energy levels can be degenerate [1 mark]

Select one:

- True
- False ✓

The correct answer is 'False'.

Question 4

Partially correct

Mark 4.00 out of 6.00

Flag question

The Huckel M.O. energies for 1,3-butadiene are: $E_1 = \alpha + 1.62\beta, E_2 = \alpha + 0.62\beta, E_3 = \alpha - 0.62\beta, E_4 = \alpha - 1.62\beta$

The corresponding M.O.s, which are linear combinations of the A.O.s are given as:

$$\phi_1 = 0.372\chi_1 + 0.602\chi_2 + 0.602\chi_3 + 0.372\chi_4,$$

$$\phi_2 = 0.602\chi_1 + 0.372\chi_2 - 0.372\chi_3 - 0.602\chi_4,$$

$$\phi_3 = 0.602\chi_1 - 0.372\chi_2 - 0.372\chi_3 + 0.602\chi_4,$$

$$\phi_4 = 0.372\chi_1 - 0.602\chi_2 + 0.602\chi_3 - 0.372\chi_4$$

a. The HOMO has ✓ nodes, while the LUMO has ✓ nodes. [1+1 marks]b. If you use the value of $\beta = -75\text{ kJ mol}^{-1}$, the resonance stabilization energy is ✗ kJ mol^{-1} . (Hint: the stabilization of ethene due to π bond formation is -150 kJ mol^{-1}) [2 marks]

c. 1,3-butadiene has a non-bonding M.O.

- True
- False ✓

The correct answer is: False

[1 mark]

c. Electrophilic substitution in 1,3-butadiene are preferred at the central carbon atoms.

- True
- False ✓

The correct answer is: False

[1 mark]

Question 5

Correct

Mark 1.00 out of 1.00

Flag question

In the variation method, the variation function must be an eigenfunction of the Hamiltonian [1 mark]

Select one:

- True
- False ✓

The correct answer is 'False'.

Question 6

Correct

Mark 1.00 out of 1.00

Flag question

If we do not ignore the overlap of the two 1s orbitals on the two H-atoms, the antibonding M.O. is more destabilized than the bonding M.O. in case of H_2^+ molecular ion [1 mark]

Select one:

- True ✓
- False

The correct answer is 'True'.

Question 7

Correct

Mark 8.00 out of 8.00

Flag question

A H-atom is in the state given by,

$$\psi = \frac{1}{81\sqrt{\pi}} \left(\frac{1}{a_0}\right)^{3/2} \left(\frac{6r}{a_0} - \frac{r^2}{a_0^2}\right) e^{-r/3a_0} \sin(\theta) [\cos(\phi) + i \sin(\phi)]$$

a. Write the values of n ✓, l ✓, $|m_l|$ ✓ [1+1+1 marks]b. ψ is an eigenfunction of \hat{L}_z . The eigenvalue, in units of \hbar , is

- [-2] [-1] 0 [+1] ✓ [+2]

The correct answer is: [+1]

[1 mark]

c. The number of radial nodes are

- 0 1 ✓ 2 3

The correct answer is: 1

[1 mark]d. The angular node is at θ equal to ✓ degrees [1 mark]

e. A transition can possibly occur to

- 2p 4f 4d ✓

The correct answer is: 4d

[1 mark]f. The ionization energy of this atom in eV is ✓ [1 mark]**Question 8**

Incorrect

Mark 0.00 out of 1.00

Flag question

One can simultaneously measure the momentum and energy of a particle in a confined particle in a box to arbitrary precision [1 mark]

Select one:

- True
- False ✗

The correct answer is 'True'.