

Chem 4A, Fall 2006
Midterm Exam 2, October 20, 2006.
Prof. Head-Gordon, Prof. Moretto

Name: GRADING KEY TA: _____

Grade:

1. (8 points)	_____
2. (5 points)	_____
3. (6 points)	_____
4. (6 points)	_____
Total:	<u>25</u>

Closed book exam. There are 6 pages. Calculators are OK. Set brains to wavelength for stimulated emission of knowledge and go! Use back side of pages for scribble paper

Some possibly useful facts and figures:

$$\begin{aligned}R &= 8.3145 \text{ J mol}^{-1} \text{ K}^{-1} \\h &= 6.6261 \times 10^{-34} \text{ J s} \\c &= 2.9979 \times 10^8 \text{ m s}^{-1} \\m_e &= 9.1094 \times 10^{-31} \text{ kg} \\N_0 &= 6.0221 \times 10^{23} \text{ mol}^{-1}\end{aligned}$$

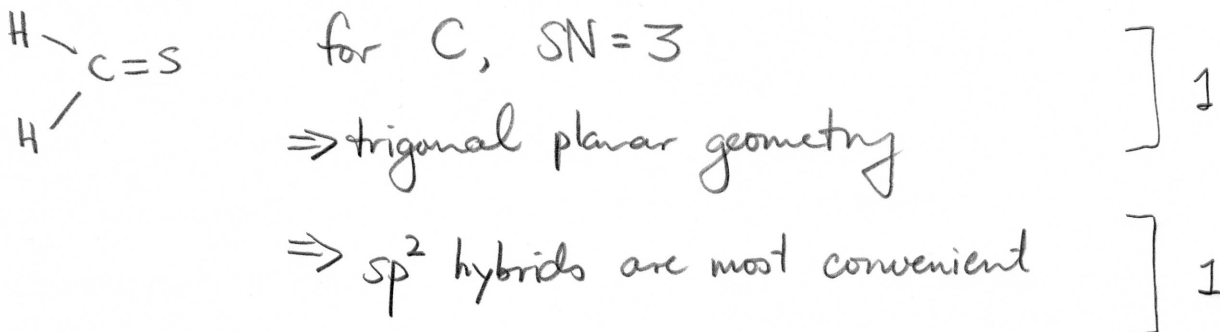
$$\begin{aligned}\text{molar volume at STP} &= 22.4 \text{ L} \\ \hbar &= h / 2\pi \\ k_B &= 1.38066 \times 10^{-23} \text{ J K}^{-1} \\ 1 \text{ atm} &= 101325 \text{ Pa}\end{aligned}$$

Some possibly relevant equations:

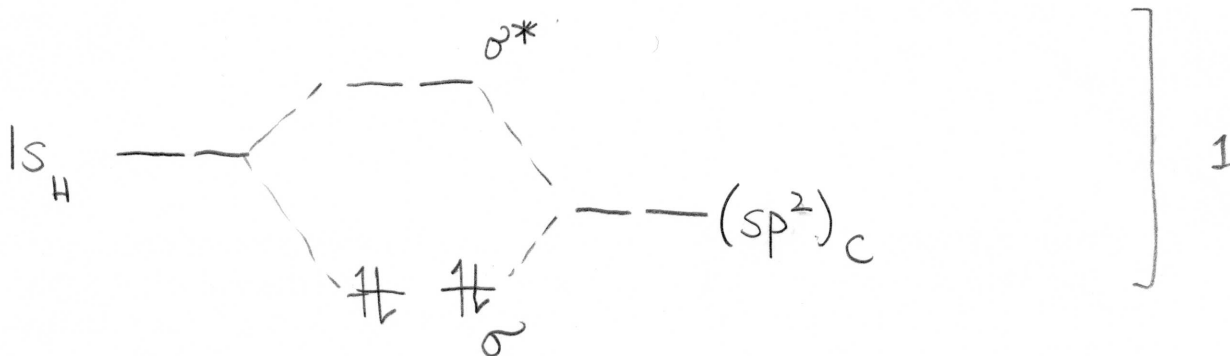
Planck relation:	$E = h\nu$	
kinetic energy	$T = \frac{1}{2}mv^2$	
diatomic rotational energies	$E_J = \frac{h^2}{8\pi^2 I} J(J+1)$	degeneracy $g_J = 2J+1$
moment of inertia	$I = \mu r^2$	
reduced mass of a diatomic	$\mu = \frac{m_1 m_2}{m_1 + m_2}$	
harmonic oscillator frequency	$\nu = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}}$	

1. (8 points) Molecular orbitals for the electrons in thioformaldehyde, $\text{H}_2\text{C}=\text{S}$.

(a) (2 points) Predict the geometry of the molecule using the VSEPR method. What kind of hybrid orbitals will you use on the C ($Z=6$) and S ($Z=16$) atoms to most conveniently predict the molecular orbitals?



(b) (2 points) Sketch the shape (boundary surface) of the 4 molecular orbitals (σ and σ^*) that describe interactions between C and the 2 H atoms. Also draw an energy level diagram showing the AO and MO energies, and which MO's are occupied.



(it's OK to just draw one of each...)



