

# INDIAN INSTITUTE OF SCIENCE EDUCATION & RESEARCH MOHALLI

CHM 201, 1<sup>st</sup> Mid Semester Examination September 10, 2018

Attempt all questions. Total number of questions: 5

2. Show clearly all the steps in your calculations.

Time: 1 hour

Total Marks: 25

## Useful data

$h = 6.626 \times 10^{-34} \text{ Js}$	$m(^{12}\text{C}) = 12.000 \text{ u}$
$c = 2.997925 \times 10^8 \text{ ms}^{-1}$	$m(^1\text{H}) = 1.008 \text{ u}$
$k = 1.380650 \times 10^{-23} \text{ JK}^{-1}$	$m(^{14}\text{N}) = 14.007 \text{ u}$
$R = 8.314472 \text{ Jmol}^{-1}\text{K}^{-1}$	$m(^{35}\text{Cl}) = 34.969 \text{ u}$
$N = 6.022142 \times 10^{23} \text{ mol}^{-1}$	$m(^{16}\text{O}) = 15.999 \text{ u}$
$1\text{eV} = 8065.479 \text{ cm}^{-1} = 23.06 \text{ kcal/mol} = 1.6021892 \times 10^{19} \text{ J}$	

- The microwave spectrum of  $^{12}\text{C}^{14}\text{N}$  observed from a certain source, shows the strongest intensity for the  $J=9 \rightarrow J=10$  transition. Given that the C-N bond length is  $1.17 \text{ \AA}$ , estimate the temperature of the source. (5)
- Smith et al. performed an infrared spectroscopy analyses of the vibrational transitions in  $^{12}\text{C}^{16}\text{O}$  and reported the value of the vibrational frequency to be  $1.302 \times 10^4 \text{ Hz}$ . a) Express the vibrational frequency in units of  $\text{cm}^{-1}$ . (2)  
 Watson et al. performed a microwave spectroscopy analyses of the rotational transitions of  $^{12}\text{C}^{16}\text{O}$  and arrive at the following equation for the energies of the rotational levels,  $E_J$ :  

$$E_J = 1.931 [J(J+1)] - 6.116 \times 10^{-6} [J(J+1)]^2$$
 b) Do you think that the data obtained from the microwave (Watson et al.) and infrared experiments (Smith et al.) are consistent with each other or not? Justify your answer. (3)
- Classify the following molecules as symmetric top, spherical top and asymmetric top. Justify your classification using symmetry arguments. (5)  
 a)  $\text{BF}_3$  b)  $\text{SF}_6$  c) m-dichlorobenzene d)  $\text{Cl}_4$  e)  $\text{CH}_2\text{Br}_2$
- The  $\text{ClO}$  diatomic species is of great importance in the chemistry of the atmosphere. A spectroscopist observed the fundamental band ( $v=0 \rightarrow v=1$ ) for the  $^{35}\text{Cl}^{16}\text{O}$  molecule at  $842.6 \text{ cm}^{-1}$ , and a hot band ( $v=1 \rightarrow v=2$ ) at  $831.6 \text{ cm}^{-1}$ .  
 a) Using the data given above, calculate  $\omega_e$  and  $\omega_e x_e$  for  $^{35}\text{Cl}^{16}\text{O}$ ? (2)  
 b) Assuming that a Morse potential adequately represents the above problem, calculate the dissociation energies,  $D_e$  and  $D_0$  for  $^{35}\text{Cl}^{16}\text{O}$ . (3)
- $\text{SiH}_4$  is a tetrahedral molecule with no dipole moment and hence cannot be expected to show a rotational spectra. However, in 1974, Rosenberg and Ozier reported the rotational spectra for this molecule (!) corresponding to transitions between  $J$  levels, involving *only large* values of  $J$ . No rotational spectra were observed for small values of  $J$ . How will you rationalize this observation? (5)