

**2021**  
**B.A./B.Sc. Semester V Honours Examination**  
**University of Calcutta**  
**CHEMISTRY**  
**Paper CC11**  
**(PRACTICAL)**  
**F.M. 30**

**FAKIR CHAND COLLEGE CENTRE (551)**

*[Use A4 pages and black ink only for writing answers. Write Roll number and Registration number at the top and page number at the bottom of each page. Images of answer script and admit card must be in a single pdf file.]*

*The figures in the margin indicate full marks.*  
(All calculations can be done using calculator)

1. Write down a Fortran Programme for determination of the value of  $\Delta S$  by using numerical integration by using both Trapezoidal rule and Simpson  $1/3$  rule.

(a) Write down the theory using the following points:

- (i) Define  $\Delta S$  for a finite change in temperature at constant pressure.
- (ii) Between  $\Delta S$  and  $\Delta G$ , which thermodynamic parameter is better in determination of chemical equilibrium and why?
- (iii) Principle of Trapezoidal rule and Simpson's  $1/3$  rule and their expressions.

2+2+3+3

- (b) Write down the FORTRAN program applying Simpson's  $1/3$  rule (in your answer script) to determine the value of  $\Delta S$  when one mole of  $O_2$  (g) is heated at constant pressure from 300K to 1200K. The constant pressure molar heat capacity of  $O_2$  (g) is

$$C_p(T) / J.K^{-1} mol^{-1} = 24.79 + (13.58 \times 10^{-3} K^{-1}) T - (37.96 \times 10^{-7} K^{-2}) T^2 \quad 14$$

- (c) If the same program is written using Trapezoidal rule what will be the Function Subprogram part? (Write only Function Subprogram part not the full FORTRAN program) 2

- (d) Calculate the value of  $\Delta S$  in your script using calculator for the above problem. 4

**N.B.: You need not to compile and run the program in computer**