Mathematics for Chemistry: Assignment 3

June 12, 2017

1. A unit positive charged particle fixed at the origin attracts a negatively charged particle at a point $\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$ by a force given by $\hat{F} = -1/r^2\hat{r}$, where $\hat{r}$ is a unit vector pointing radially outwards. The work done in moving the particle from a point (1,1,2) to a point (0,2,2) along a straight line is closest to
   (a) -0.5 (b)-0.71 (c)-0.29 (d) 0
   Answer (c)

2. The work done by the force $\hat{F}(x, y) = 3(x/y)\hat{i} + (x^2 + y^2)\hat{j}$ in moving a particle from (1,0) to (-1,0) counterclockwise along a circular path of radius 1 is equal to
   (a) -2 (b) 0 (c) + 2 (d) 2/3
   Answer (b)

3. Consider the three forces below:
   (A) $2x^2\hat{i} + 4xy\hat{j}$
   (B) $4xy\hat{i} + 2x^2\hat{j}$
   (C) $4(x/y)\hat{i} + 4(y/x)\hat{j}$
   The forces which are conservative are

   (a) A,B and C
   (b) B and C but not A
   (c) B only
   (d) C only

   Answer (c)

4. The differential work done dW in expanding a gas reversibly is given as $-PdV$ where P is the pressure and dV represents the change in volume. The work done in expanding a gas from an initial pressure of 10^5 Pa and initial volume of 1 L to a final pressure of 0.5×10^5 Pa and final volume of 2 L along a straight line path (in P-V space) is equal to (in J)
   (a) 100 (b) 75 (c) 40 (d) 200
   Answer (b)

5. According to the first two laws of thermodynamis, we have the change in Gibbs free energy dG related to the change in pressure dP and the change in temperature dT via $dG(P, T) = V(P, T)dP - S(P, T)dT$. The condition for $G(P, T)$ to be an exact differential gives the relation

   (a)
   $$\frac{\partial V}{\partial P} = \frac{\partial S}{\partial T}$$

   (b)
   $$\frac{\partial V}{\partial P} = -\frac{\partial S}{\partial T}$$

   (c)
   $$\frac{\partial V}{\partial T} = -\frac{\partial S}{\partial P}$$

(d)

$$\frac{\partial V}{\partial T} = -\frac{\partial S}{\partial P}$$

Answer (c)

6. According to the first two laws of thermodynamics, we have the change in Gibbs free energy dG related to the change in pressure dP and the change in temperature dT via $dG(P,T) = V(P,T)dP - S(P,T)dT$. Additonally we are given $V = RT/P$ where R is a constant. The expression for S is

   (a) $S = R + C$ where C is a constant independent of T and P.

   (b) $S = -R + C$ where C is a constant independent of T and P.

   (c) $S = R \ln P + f(T)$ where $f(T)$ is a function of T only.

   (d) $S = -R \ln P + f(T)$ where $f(T)$ is a function of T only.

   Answer (d)

7. According to the first two laws of thermodynamics, we have the change in Helmholtz free energy dA related to the change in pressure dV and the change in temperature dT via $dA = -(RT/V)dV - (R\ln(V) + 3R/2T)dT$, where V is expressed in some units. The work done in changing the state of the system from an initial volume 1 and temperature 1 (in some units) to a final volume 2 and temperature 2 is equal to
   (a) 0 (b) $3R/2$ (c)$7R/2$ (d) $(7R/2)\ln 2$

   Answer (d)

8. The surface integral over the surface of a sphere of radius 1 of the vector field $\hat{V} = x\hat{i} + y\hat{j} + z\hat{k}$ is equal to
   (a) 0 (b) π (c) 2π (d) 4π
   Answer (d)

9. The wave function of a particle in a 3D rectangular box located between $x = 0$ to $x = 1$, $y = 0$ to $y = 2$ and $z = 0$ to $z = 2$ is proportional to $\sin(\pi x)\sin(\pi y/2)\sin(\pi z/2)$. The volume integral of the *square* of this function inside the box is equal to
   (a) 1 (b) 1/2 (c) 2 (d) 4
   Answer (c)

10. The wave function of an electron in the Hydrogen atom in the 2p$_z$ orbital in spherical polar coordinates is proportional to $\cos\theta(r/a_0)e^{-r/2a_0}$ where a_0 is a constant. The volume integral of the *square* of this function over all space is equal to (use the result $\int_0^\infty x^n e^{-x}dx = n!$)
    (a) $32\pi a_0^3$ (b) $4\sqrt{2\pi}a_0^{3/2}$ (c) $\frac{1}{32\pi a_0^3}$ (d)$\frac{1}{4\sqrt{2\pi}a_0^{3/2}}$
    Answer (a)