Unit 7 - Week 6:

Assignment 6

1) The coefficient of x^2 in the Taylor expansion of the function f(x) given by $f(x) = \frac{1}{\sqrt{1+x^2}}$ is **1** point equal to

1 3 0 None of the above

Accepted Answers:

2) The radial part of the wavefunction of the a 3d electron in the hydrogen atom is given by $R_{3d}(r) \propto r^2 \exp(-r/3a_0)$. The maximum value of the radial probability distribution, $P(r) = r^2(R_{3d}(r))^2$, is obtained at a value of r/a_0 of

```
1
3
9
None of the above
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Accepted Answers:

9

3) The Van der Waals equation of state for a gas at some temperature relates the pressure p **1** point and molar volume v via

$$(p + \frac{a}{v^2})(v - b) = \frac{4aR}{27b}$$

where *a*, *b*, *R* are positive constants. In this case, the number of extrema of in the p-v graph is

Accepted Answers: 3 4) Consider the Van der Waals equation of a gas at some temperature given by 1 point $(p + \frac{a}{v^2})(v - b) = \frac{8aR}{27b}$ where p is the pressure of the gas, v is the molar volume, and a, b, R are positive constants. The saddle point of this equation is obtained for a value of v of 0 h 3b None of the above **Accepted Answers:** 3b5) Consider the Taylor series expansion of the function sin(xy) about the point (0,0). The 1 point coefficient of xy in the expansion is 0 1 2 1/2 **Accepted Answers:** 1 6) Consider a two-dimensional potential energy surface of the form 1 point $V(x, y) = xy - x^2y^2 + 0.25(x^2 + y^2) + 0.125(x^4 + y^4)$

The point (1,1) is a

- maximum in all directions.
- minimum in all directions.
- saddle point.
- None of the above.

Accepted Answers:

saddle point.

7) The Hessian of the potential energy function $V(x, y) = xy - 0.25x^2y^2 + 0.25(x^2 + y^2)$ **1** point at (0,0) is equal to

-0.75
 -0.25
 0
 None of the above

Accepted Answers: -0.75

Advance

ed	Mathematical Methods for Chemistry Unit 7 - Week 6: Optimization, Constrained Optimization	
	8) The maximum value of the function $f(x, y) = 2x - 3y$ on the circle $x^2 + y^2 = 13$ is equal 1	point
	to	
	O 4	
	09	
	13	
	None of the above	
	Accepted Answers:	
	13	
	9) The number of saddle points of the function $x^3 + y^2 - 3x - 3y$ is 1)	ooint
	O 0	
	0 1	
	2	
	3	
	Accepted Answers:	
	2	
	10) The shape of a parallelopiped (sides a, b, c) with the 1	point
	maximum area ($2(ab + bc + ca)$) for a	
	fixed perimeter $(4(a + b + c))$ is	
	a cube	
	a square based cuboid but not a cube	
	a cuboid with all three dimensions different	
	something that cannot be determined from the above information	
	Accepted Answers:	
	a cube	