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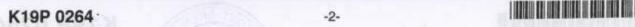
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II	Semester M.Sc. Degree (Reg./Suppl./Imp.) Examination, April 2019 (2014 Admission Onwards) CHEMISTRY CHE 2C05: Theoretical Chemistry – II
Tim	ne : 3 Hours Max. Marks : 6
1 1111	SECTION - A Canil as anti-stokes lines 7 A - NOITOS
	nswer all questions each in one word or sentence. Each question carries mark:
1.	What is identity element?
2.	What is order of a group ?
3.	What is a character?
4.	In a given representation, the character of all matrices belonging to operations in the same class are
5.	In hydrogen molecule, when hydrogen is replaced by Deuterium, what will happen to the rotational constant, B?
6.	What is transition moment integral?
7.	Which transition has the smallest molar absorptivity?
	a) $\pi - \pi^*$ b) $\sigma - \sigma^*$ c) $n - \pi^*$ d) $\sigma - \pi^*$
8.	Write down the value of nuclear spin in <sup>19</sup> F and <sup>31</sup> P. (8×1=8
	SECTION - B

Answer eight questions. Answer may be in two or three sentences.

Each question carries 2 marks:

- 9. Prove that the order of any subgroup 'g' of a group of order 'h' must be a divisor of 'h'.
- 10. Define similarity transformation.

P.T.O.



- 11. What is an abelian group?
- 12. Differentiate between reducible and irreducible representation.
- Differentiate between operator E and Mulliken symbol, E.
- 14. Name the various regions of electromagnetic spectrum.
- 15. What are the selection rules in IR spectroscopy?
- 16. What is Doppler broadening?
- 17. What are anti-stokes lines?
- 18. Write the effect of solvents in electronic transition.
- 19. What is TMS? What is its use in NMR spectroscopy?
- Define nuclear magneton.

 $(8 \times 2 = 16)$ 

## SECTION - C

Answer four questions each in one paragraph. Each question carries 3 marks :

- 21. What are the conditions that must be satisfied by any set of elements to form a mathematical group?
- 22. Construct a representation for Pz orbital on the oxygen atom of H<sub>2</sub>O.
- 23. Determine the hybridization in BF<sub>3</sub> using the D<sub>3h</sub> character table given below.

D <sub>3h</sub>	Е	2C <sub>3</sub>	3C <sub>2</sub>	$\sigma_{h}$	2S <sub>3</sub>	<b>3</b> σ <sub>v</sub>	eliama eri	carl millerish has
A1'	1	1	1	1	1	1	70-0	$x^2+y^2, z^2$
A2'	1	1	- 1	1	1	- 1	R <sub>z</sub>	nulsy aft myob
E'	2	- 1	0	2	- 1	0	(x, y)	$(x^2 - y^2, xy)$
A1"	1	1	1	- 1	-1	-1		
A2"	1	261191	-1	-1	-1	ad1/s	Z	ight questions
E"	2	-1	0	-2	1	0	$(R_x, R_y)$	(xz, yz)

- 24. What are the rules in assigning Mulliken symbols to various representations?
- 25. The first line in the rotational spectrum of CO has a frequency of 3.8424 cm<sup>-1</sup>. Calculate the rotational constant and hence the C-O bond length.

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26. Give an account of how Raman spectrum gives valuable information about molecular structure.

27. Explain the factors affecting chemical shift.

28. Explain spin-lattice relaxation.

 $(4 \times 3 = 12)$ 

## SECTION - D

Answer either A or B of each question. Each question carries 6 marks :

 A) Construct the reducible representation for H<sub>2</sub>O molecule from the Cartesian co-ordinates of atoms.

OR

B) i) Assign the point groups to following molecules and justify : eclipsed ethane, staggered ethane, benzene.

ii) Explain with examples improper axis and improper rotation. What are the different kinds of operations generated by Sn (n = odd and even) operation?

 A) State and explain Great Orthogonality Theorem. Also, discuss the important rules about irreducible representations and their characters.

OR

- B) Derive the character table for C<sub>3</sub>v.
- 31. A) Explain the rule of mutual exclusion. Sketch and explain the polarisability ellipsoids of various modes of vibration of CO<sub>2</sub> molecule. Which of these are Raman active?

OR

- B) Discuss vibrational coarse structure or progressions.
- A) With the help of Franck-Codon principle, illustrate the shapes of the absorption bands.

OR

B) What is coupling constant? Explain the effect of coupling between two neighboring nuclei on the splitting pattern of their NMR signals. (4x6=24)