Roll No. .....

Question Booklet Number

O. M. R. Serial No.

M. Sc. (Fourth Semester)

(NEP) EXAMINATION, 2025-26

CHEMISTRY

(Computational Chemistry)

Paper Code							
B	0	2	1	0	0	7	T

Questions Booklet Series
B

Time : 1:30 Hours] [*Maximum Marks : 75*

Instructions to the Examinee :

1. Do not open the booklet unless you are asked to do so.

2. The booklet contains 100 questions. Examinee is required to answer 75 questions in the OMR Answer-Sheet provided and not in the question booklet. All questions carry equal marks.

3. Examine the Booklet and the OMR Answer-Sheet very carefully before you proceed. Faulty question booklet due to missing or duplicate pages/questions or having any other discrepancy should be got immediately replaced.

परीक्षार्थियों के लिए निर्देश :

1. प्रश्न-पुस्तिका को तब तक न खोलें जब तक आपसे कहा न जाए।

2. प्रश्न-पुस्तिका में 100 प्रश्न हैं। परीक्षार्थी को 75 प्रश्नों को केवल दी गई OMR आन्सर-शीट पर ही हल करना है, प्रश्न-पुस्तिका पर नहीं। सभी प्रश्नों के अंक समान हैं।

3. प्रश्नों के उत्तर अंकित करने से पूर्व प्रश्न-पुस्तिका तथा OMR आन्सर-शीट को सावधानीपूर्वक देख लें। दोषपूर्ण प्रश्न-पुस्तिका जिसमें कुछ भाग छपने से छूट गए हों या प्रश्न एक से अधिक बार छप गए हों या उसमें किसी अन्य प्रकार की कमी हो, तो उसे तुरन्त बदल लें।

(Remaining instructions on the last page) (NEW) **(शेष निर्देश अन्तिम पृष्ठ पर)**

(Only for Rough Work)

1. The 'logical' data type in Fortran can have values :

(A) 0 and 1

(B) .TRUE. and .FALSE.

(C) YES and NO

(D) T and F

2. Truncation error in Taylor series occurs because :

(A) We omit higher-order terms of the series

(B) We round off numbers

(C) The computer hardware is slow

(D) The user made a typo

3. The 'Newton-Cotes' formulas are used for :

(A) Finding roots

(B) Numerical integration

(C) Sorting arrays

(D) Finding eigenvalues

4. GAUSSIAN uses 'Gaussian-type orbitals' (GTOs) because :

(A) They are physically accurate

(B) They are larger

(C) They are computationally easier to integrate than Slater-type orbitals (STOs)

(D) They don't require energy

5. Which method is 'self-starting' for solving ODEs ?

(A) Adams-Bashforth

(B) Taylor series expansion beyond first term

(C) Predictor-Corrector

(D) Runge-Kutta

6. In C, '++*i*' is known as :

(A) Post-increment

(B) Pre-increment

(C) Addition

(D) Pointer

7. The 'pivoting' strategy in Gaussian Elimination helps minimize :

(A) Round

(B) Offerrors Logical

(C) Errors

(D) Memory usage

8. Gaussian 09 or 16 output files usually have the extension :

(A) .exe

(B) .log *or* .out

(C) .png

(D) .mp3

9. Which semi-empirical method is part of MOPAC ?

(A) B3LYP

(B) CCSD(T)

(C) MP2

(D) AM1 or PM6

10. The 'Polynomial Wiggle' can be reduced by using :

(A) Higher degree polynomials

(B) Spline interpolation (piecewise polynomials)

(C) Bisection

(D) Gaussian elimination

11. In a networking context, DNS stands for :

(A) Data Network System

(B) Digital Node Server

(C) Domain Name System

(D) Direct Network Search

12. Numerical differentiation using forward difference is :

(A) First-order accurate

(B) Second-order accurate

(C) Fourth-order accurate

(D) Perfectly accurate

13. The 'Hartree-Fock' method is a :

(A) Semi-empirical method

(B) Ab initio method

(C) Molecular mechanics method

(D) Statistical averaging

14. The C library function 'pow(x, y)' is found in :

(A) <stdio.h>

(B) <conio.h>

(C) <stdlib.h>

(D) <math.h>

15. A Fortran 'MODULE' is used for :

(A) Deleting files

(B) Encapsulating data and subroutines

(C) Printing text

(D) Calculating square roots

16. Errors in Romberg integration are associated with :

(A) The step size 'h'

(B) The speed of the CPU

(C) The number of variables

(D) The color of the GUI

17. Which is NOT a valid molecular docking software ?

(A) AutoDock

(B) GOLD

(C) Photoshop

(D) Glide

18. The 'force field' in AMBER consists of :

(A) Magnetic fields

(B) Potential energy functions for bonds, angles and dihedrals

(C) Electric currents

(D) Gravitational constants

19. Convergence in Gauss-Seidel is faster if the matrix is :

(A) Small

(B) Diagonally dominant

(C) Singular

(D) Symmetric only

20. The 'Hermite' interpolation polynomial matches both :

(A) Function values and slopes

(B) Function values and integrals

(C) Slopes and curvature

(D) Value sat infinity

21. Ab initio packages like GAMESS are often written in :

(A) HTML

(B) FORTRAN/C++

(C) Python only

(D) Java

22. What is the limit of 'h' in the definition of a derivative ?

(A) $h \to 1$

(B) $h \to \infty$

(C) $h \to 0$

(D) $h \to -1$

23. Matrix diagonalization of the Hamiltonian matrix gives :

(A) Atomic coordinates

(B) Dipole moments

(C) Bond lengths

(D) Energy eigenvalues

24. Central difference formula for differentiation is more accurate than :

(A) Backward difference

(B) Forward difference

(C) Both (A) and (B)

(D) Neither

25. The efficiency of a program is often measured by its :

(A) File size

(B) Time and Space complexity

(C) Variable names

(D) Number of comments

26. In networking, a 'Router' is used to :

(A) Forward data packets between computer networks

(B) Create web pages

(C) Type code

(D) Cool the CPU

27. 'Convergence' in a numerical method means :

(A) The values are getting larger

(B) The sequence of values approaches the true solution

(C) The computer has stopped working

(D) The program has finished

28. Simpson's 3/8 rule is more accurate than Simpson's 1/3 rule for :

(A) Linear functions

(B) Finding roots

(C) Certain higher-order polynomials

(D) All functions

29. Structure-Activity Relationship (SAR) helps in :

(A) Synthesis of chemicals

(B) Understanding how structural features affect biological response

(C) Naming molecules

(D) Measuring density

30. GAUSSIAN exercises for students often start with :

(A) Full protein folding

(B) Breaking the internet

(C) Simulating a nuclear explosion

(D) Geometry optimization of simple molecules like water or methane

31. Newton's backward difference formula uses data points :

(A) x_n, x_{n-1}, x_{n-2}...

(B) x_0, x_1, x_2...

(C) Randomly

(D) Only the first two

32. In C, a 'pointer' stores :

(A) An integer value

(B) A memory address

(C) A character

(D) A floating point number

33. Regular Falsi is generally :

(A) Faster than Newton-Raphson

(B) Not a root-finding method

(C) Slower than Newton-Raphson but more reliable in convergence

(D) Used only for linear equations

34. Matrix ill-conditioning is checked using the :

(A) Trace

(B) Condition Number

(C) Rank

(D) Size

35. MOPAC is most useful for :

(A) Small atoms like Helium

(B) Browsing the web

(C) Calculating the weight of a beaker

(D) Large organic molecules where ab initio is too slow

36. In Fortran, the 'IMPLICIT NONE' statement :

(A) Speeds up the program

(B) Forces the explicit declaration of all variables

(C) Is optional and rarely used

(D) Declares all variables as integers

37. Numerical integration is also called :

(A) Numerical Quadrature

(B) Numerical Rooting

(C) Numerical Solving

(D) Numerical Factoring

38. The error in the Trapezoidal rule is of the order :

(A) $O(h)$

(B) $O(h^2)$

(C) $O(h^4)$

(D) $O(1)$

39. Ab initio methods solve the :

(A) Electronic Schrödinger Equation

(B) Ideal Gas Equation

(C) Stock Market Equation

(D) Maxwell's Equations

40. A firewall in networking is used for :

(A) Monitoring temperature

(B) Speeding up the mouse

(C) Security/Filtering unauthorized access

(D) Deleting spam

41. In numerical methods, 'Local Truncation Error' refers to the error :

(A) Over the entire calculation

(B) In a single step of the method

(C) Due to typing

(D) From the sensor

42. Which is a 'Predictor-Corrector' method ?

(A) Bisection

(B) Jacobi Method

(C) Gaussian Elimination

(D) Milne's Method

43. Lagrange polynomials do not require :

(A) Function values

(B) Equally spaced intervals

(C) Variable x

(D) A computer

44. Gauss-Jordan elimination is used to find the :

(A) Inverse of a matrix

(B) Root of an equation

(C) Derivative

(D) Integral

45. Quantum chemical packages calculate 'Total Energy' by :

(A) Adding atomic weights

(B) Summing kinetic and potential energy terms of electrons and nuclei

(C) Using a thermometer

(D) Guessing

46. Searching scientific literature on the internet often uses :

(A) Boolean operators (AND, OR, NOT)

(B) Only emojis

(C) Facebook

(D) Fortran

47. III-conditioning in interpolation happens when :

(A) Points are too far apart

(B) Using C instead of Fortran

(C) The function is a constant

(D) Points are too close together relative to precision

48. Double precision in Fortran/C provides approximately :

(A) 7 decimal digits

(B) 30 decimal digits

(C) 15-16 decimal digits

(D) 2 decimal digits

49. The Schrödinger equation is a :

(A) Linear algebraic equation

(B) Partial differential equation

(C) Quadratic equation

(D) Integral equation

50. Internet search results are ranked using :

(A) Algorithms (like PageRank)

(B) Human voting

(C) Alphabetical order

(D) Random selection

51. Which feature in C allows a function to call itself ?

(A) Iteration

(B) Recursion

(C) Inline expansion

(D) Nesting

52. In Fortran, which statement is used to define a custom data type ?

(A) struct

(B) record

(C) class

(D) type

53. The 'ill-conditioning' of a mathematical problem refers to :

(A) Poor programming logic

(B) High sensitivity of the solution to small changes in input data

(C) Lack of computer memory

(D) Using the wrong compiler

54. Round-off error in numerical methods typically occurs due to :

(A) Finite precision of floating-point representation

(B) Using too many iterations

(C) Simplifying the physical model

(D) Incorrect initial guesses

55. Which C operator is used to access the memory address of a variable ?

(A) *

(B) ->

(C) &

(D) .

56. The Bisection method is guaranteed to converge if :

(A) The function is a polynomial

(B) The function is continuous and changes sign over the interval

(C) The initial guess is close to the root

(D) The derivative of the function is known

57. What is the rate of convergence for the Newton-Raphson method ?

(A) Linear

(B) Cubic

(C) Quadratic

(D) Logarithmic

58. In solving the van der Waals equation for molar volume, the Newton-Raphson method fails if :

(A) The initial guess for Volume results in $f'(V) = 0$

(B) The pressure is too high

(C) The gas is ideal

(D) The temperature is above the critical point

59. The Regula-Falsi method is also known as :

(A) Method of tangents

(B) Method of false position

(C) Interval halving

(D) Steepest descent

60. A transcendental equation is an equation that :

(A) Contains only polynomials

(B) Cannot be solved numerically

(C) Has only complex roots

(D) Involves trigonometric, exponential, or logarithmic functions

61. Gaussian elimination transforms the coefficient matrix into :

(A) A diagonal matrix

(B) An upper triangular matrix

(C) An identity matrix

(D) A lower triangular matrix

62. The Gauss-Seidel method is an example of :

(A) A direct method

(B) A recursive method

(C) An iterative method

(D) A symbolic method

63. In Gaussian elimination, 'pivoting' is performed to :

(A) Speed up the calculation

(B) Avoid division by zero or very small numbers

(C) Reduce the number of variables

(D) Transform the matrix to its transpose

64. The Gauss-Jordan method results in the matrix becoming :

(A) Upper triangular

(B) Lower triangular

(C) Reduced row echelon form (Identity)

(D) Singular

65. Which method is most efficient for solving large sparse systems often found in molecular simulations ?

(A) Cramer's Rule

(B) Gaussian Elimination

(C) Gauss-Seidel

(D) Gauss-Jordan

66. Jacobi's method is used for finding eigenvalues of :

(A) Any square matrix

(B) Singular matrices

(C) Only 2×2 matrices

(D) Symmetric matrices

67. Matrix diagonalization is essential in Quantum Chemistry for :

(A) Finding the molecular weight

(B) Solving the Schrödinger equation for energy levels

(C) Balancing chemical equations

(D) Calculating boiling points

68. The Householder method reduces a symmetric matrix to :

(A) Diagonal form

(B) Identity form

(C) Tridiagonal form

(D) Triangular form

69. An eigenvalue of a matrix A satisfies the equation :

(A) $\det(A - \lambda I) = 0$

(B) $A\lambda = I$

(C) $\det(A) = \lambda$

(D) $A + \lambda I = 0$

70. Which numerical error is most critical during repeated matrix transformations in Jacobi's method ?

(A) Truncation error

(B) Accumulation of round-off errors

(C) Modeling error

(D) User input error

71. Newton's forward difference formula is best used for points :

(A) Near the end of a data set

(B) Outside the range of data

(C) In the middle of a data set

(D) Near the beginning of a data set

72. Lagrange interpolation is preferred over Newton's formula when :

(A) Data points are equally spaced

(B) The polynomial degree is very high

(C) Data points are unequally spaced

(D) Only two points are given

73. The 'Polynomial Wiggle' (Runge's Phenomenon) occurs when :

(A) The degree of the interpolating polynomial is too low

(B) High-degree polynomials are used for interpolation over equidistant points

(C) The data contains no errors

(D) The function is linear

74. Hermite interpolation requires knowledge of both function values and :

(A) Second derivatives

(B) Integration constants

(C) First derivatives (slopes)

(D) Eigenvalues

75. In chemistry, interpolation is commonly used to :

(A) Find values between experimental data points in a table (e.g., vapor pressure)

(B) Solve a rate law

(C) Balance a redox reaction

(D) Define a new element

76. The Runge-Kutta 4th order method is used to solve :

(A) Algebraic equations

(B) Ordinary differential equations (ODEs)

(C) Integrals only

(D) Partial differential equations only

77. Simpson's 1/3 rule for integration requires the number of intervals to be :

(A) Odd

(B) A multiple of 3

(C) A prime number

(D) Even

78. Newton-Cotes formulas approximate the integral of a function using :

(A) Tangent lines

(B) Polynomials

(C) Logarithms

(D) Sine waves

79. Romberg integration is based on :

(A) Richardson extrapolation of the Trapezoidal rule

(B) Bisection

(C) Gaussian elimination

(D) Taylor series only

80. Numerical differentiation of experimental data is highly sensitive to :

(A) The number of significant figures

(B) The color of the solution

(C) Noise/scatter in the data

(D) Atmospheric pressure

81. Which package is primarily used for ab initio quantum chemical calculations ?

(A) AMBER

(B) GAUSSIAN

(C) CHARMM

(D) QUANTA

82. Semi-empirical methods like MOPAC are faster than ab initio because :

(A) They ignore electrons

(B) They don't use the Schrödinger equation

(C) They only work on hydrogen

(D) They use experimental parameters to approximate certain integral

83. Molecular Dynamics (MD) simulations in AMBER use :

(A) Classical Force Fields

(B) Pure Wave functions

(C) Only Lewis structures

(D) Titration curves

84. QSAR (Quantitative Structure-Activity Relationship) is used in :

(A) Identifying isotopes

(B) Predicting biological activity of drug candidates

(C) Calculating molar mass

(D) Designing glass apparatus

85. The primary purpose of the 'GAUSSIAN' package in computational chemistry is :

(A) To manage laboratory inventory

(B) To draw 2D chemical structures

(C) To calculate molecular structures and vibrational frequencies

(D) To simulate liquid chromato-graphy

86. Which software is specifically famous for protein and nucleic acid simulations ?

(A) CHARMM

(B) GAMESS

(C) MOPAC

(D) MATLAB

87. In computational chemistry, a 'Basis Set' is :

(A) A set of laboratory rules

(B) The initial temperature of a reaction

(C) A collection of solvents

(D) Mathematical functions used to represent atomic orbitals

88. 'Molecular Docking' (QUANTA/ CHARMM) is used to study :

(A) How a ligand binds to a receptor/protein

(B) The boiling point of a solvent

(C) The crystal structure of NaCl

(D) The diffusion of gases

89. Ab initio methods solve the Schrödinger equation :

(A) Using experimental data points

(B) From first principles without empirical data

(C) Using only Newton's laws

(D) Using only the ideal gas law

90. Simulation of transition states is critical for :

(A) Drug delivery only

(B) Determining the price of chemicals

(C) Catalyst design and reaction mechanism studies

(D) Naming organic compounds

91. What does IP stand for in networking ?

(A) Internal Process

(B) Instant Package

(C) Integrated Program

(D) Internet Protocol

92. A 'search engine' uses which of the following to index web pages ?

(A) Browsers
(B) Spiders/Crawlers
(C) Firewalls
(D) Routers

93. Which protocol is used for secure data transmission over the web ?

(A) HTTP
(B) FTP
(C) HTTPS
(D) SMTP

94. TCP/IP is a :

(A) Type of computer
(B) Suite of communication protocols
(C) Programming language
(D) Database software

95. In chemistry research, 'PubMed' *or* 'SciFinder' are examples of :

(A) Operating systems
(B) Molecular editors
(C) Computer viruses
(D) Search engines/databases for scientific literature

96. A syntax error in C is detected at :

(A) Compile time
(B) Runtime
(C) Link time
(D) Post-processing

97. FORTRAN was originally designed for :

(A) Web development
(B) Scientific and engineering calculations
(C) Database management
(D) Artificial Intelligence

98. In C, the 'float' data type generally occupies :

(A) 2 bytes
(B) 1 byte
(C) 8 bytes
(D) 4 bytes

99. Which is a valid variable name in C ?

(A) 2_molar
(B) molar_conc
(C) molar conc
(D) float

100. What is the output of 5/2 in C if both are integers ?

(A) 2.5
(B) 3
(C) 2
(D) Error

(Only for Rough Work)

4. Four alternative answers are mentioned for each question as—A, B, C & D in the booklet. The candidate has to choose the correct answer and mark the same in the OMR Answer-Sheet as per the direction :

Example :

Question :

Q. 1 (A) ● (C) (D)
Q. 2 (A) (B) ● (D)
Q. 3 (A) ● (C) (D)

Illegible answers with cutting and over-writing or half filled circle will be cancelled.

5. Each question carries equal marks. Marks will be awarded according to the number of correct answers you have.
6. All answers are to be given on OMR Answer Sheet only. Answers given anywhere other than the place specified in the answer sheet will not be considered valid.
7. Before writing anything on the OMR Answer Sheet, all the instructions given in it should be read carefully.
8. After the completion of the examination candidates should leave the examination hall only after providing their OMR Answer Sheet to the invigilator. Candidate can carry their Question Booklet.
9. There will be no negative marking.
10. Rough work, if any, should be done on the blank pages provided for the purpose in the booklet.
11. To bring and use of log-book, calculator, pager and cellular phone in examination hall is prohibited.
12. In case of any difference found in English and Hindi version of the question, the English version of the question will be held authentic.

Impt. : On opening the question booklet, first check that all the pages of the question booklet are printed properly. If there is any discrepancy in the question Booklet, then after showing it to the invigilator, get another question Booklet of the same series.

4. प्रश्न-पुस्तिका में प्रत्येक प्रश्न के चार सम्भावित उत्तर—A, B, C एवं D हैं। परीक्षार्थी को उन चारों विकल्पों में से सही उत्तर छाँटना है। उत्तर को OMR आन्सर-शीट में सम्बन्धित प्रश्न संख्या में निम्न प्रकार भरना है :

उदाहरण :

प्रश्न :

प्रश्न 1 (A) ● (C) (D)
प्रश्न 2 (A) (B) ● (D)
प्रश्न 3 (A) ● (C) (D)

अपठनीय उत्तर या ऐसे उत्तर जिन्हें काटा या बदला गया है, या गोले में आधा भरकर दिया गया, उन्हें निरस्त कर दिया जाएगा।

5. प्रत्येक प्रश्न के अंक समान हैं। आपके जितने उत्तर सही होंगे, उन्हीं के अनुसार अंक प्रदान किये जायेंगे।
6. सभी उत्तर केवल ओ. एम. आर. उत्तर-पत्रक (OMR Answer Sheet) पर ही दिये जाने हैं। उत्तर-पत्रक में निर्धारित स्थान के अलावा अन्यत्र कहीं पर दिया गया उत्तर मान्य नहीं होगा।
7. ओ. एम. आर. उत्तर-पत्रक (OMR Answer Sheet) पर कुछ भी लिखने से पूर्व उसमें दिये गये सभी अनुदेशों को सावधानीपूर्वक पढ़ लिया जाये।
8. परीक्षा समाप्ति के उपरान्त परीक्षार्थी कक्ष निरीक्षक को अपनी OMR Answer Sheet उपलब्ध कराने के बाद ही परीक्षा कक्ष से प्रस्थान करें। परीक्षार्थी अपने साथ प्रश्न-पुस्तिका ले जा सकते हैं।
9. निगेटिव मार्किंग नहीं है।
10. कोई भी रफ कार्य, प्रश्न-पुस्तिका के अन्त में, रफ-कार्य के लिए दिए खाली पेज पर ही किया जाना चाहिए।
11. परीक्षा-कक्ष में लॉग-बुक, कैलकुलेटर, पेजर तथा सेल्युलर फोन ले जाना तथा उसका उपयोग करना वर्जित है।
12. प्रश्न के हिन्दी एवं अंग्रेजी रूपान्तरण में भिन्नता होने की दशा में प्रश्न का अंग्रेजी रूपान्तरण ही मान्य होगा।

महत्वपूर्ण : प्रश्नपुस्तिका खोलने पर प्रथमतः जाँच कर देख लें कि प्रश्न-पुस्तिका के सभी पृष्ठ भलीभाँति छपे हुए हैं। यदि प्रश्नपुस्तिका में कोई कमी हो, तो कक्षनिरीक्षक को दिखाकर उसी सिरीज की दूसरी प्रश्न-पुस्तिका प्राप्त कर लें।