

Roll No.

Question Booklet Number

O. M. R. Serial No.

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M. Sc. (Fourth Semester)
(NEP) EXAMINATION, 2025-26

CHEMISTRY

(Computational Chemistry)

Paper Code						
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Questions Booklet Series
D

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. What is the output of $5/2$ in C if both are integers ?
 - (A) 2.5
 - (B) 3
 - (C) 2
 - (D) Error

2. Which is a valid variable name in C ?
 - (A) 2_molar
 - (B) molar_conc
 - (C) molar conc
 - (D) float

3. In C, the 'float' data type generally occupies :
 - (A) 2 bytes
 - (B) 1 byte
 - (C) 8 bytes
 - (D) 4 bytes

4. FORTRAN was originally designed for :
 - (A) Web development
 - (B) Scientific and engineering calculations
 - (C) Database management
 - (D) Artificial Intelligence

5. A syntax error in C is detected at :
 - (A) Compile time
 - (B) Runtime
 - (C) Link time
 - (D) Post-processing

6. 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

7. TCP/IP is a :
 - (A) Type of computer
 - (B) Suite of communication protocols
 - (C) Programming language
 - (D) Database software

8. Which protocol is used for secure data transmission over the web ?
 - (A) HTTP
 - (B) FTP
 - (C) HTTPS
 - (D) SMTP

9. A 'search engine' uses which of the following to index web pages ?
 - (A) Browsers
 - (B) Spiders/Crawlers
 - (C) Firewalls
 - (D) Routers

10. What does IP stand for in networking ?
- Internal Process
 - Instant Package
 - Integrated Program
 - Internet Protocol
11. Simulation of transition states is critical for :
- Drug delivery only
 - Determining the price of chemicals
 - Catalyst design and reaction mechanism studies
 - Naming organic compounds
12. Ab initio methods solve the Schrödinger equation :
- Using experimental data points
 - From first principles without empirical data
 - Using only Newton's laws
 - Using only the ideal gas law
13. 'Molecular Docking' (QUANTA/CHARMM) is used to study :
- How a ligand binds to a receptor/protein
 - The boiling point of a solvent
 - The crystal structure of NaCl
 - The diffusion of gases
14. In computational chemistry, a 'Basis Set' is :
- A set of laboratory rules
 - The initial temperature of a reaction
 - A collection of solvents
 - Mathematical functions used to represent atomic orbitals
15. Which software is specifically famous for protein and nucleic acid simulations ?
- CHARMM
 - GAMESS
 - MOPAC
 - MATLAB
16. The primary purpose of the 'GAUSSIAN' package in computational chemistry is :
- To manage laboratory inventory
 - To draw 2D chemical structures
 - To calculate molecular structures and vibrational frequencies
 - To simulate liquid chromatography
17. QSAR (Quantitative Structure-Activity Relationship) is used in :
- Identifying isotopes
 - Predicting biological activity of drug candidates
 - Calculating molar mass
 - Designing glass apparatus
18. Molecular Dynamics (MD) simulations in AMBER use :
- Classical Force Fields
 - Pure Wave functions
 - Only Lewis structures
 - Titration curves

19. 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
20. Which package is primarily used for ab initio quantum chemical calculations ?
- (A) AMBER
 - (B) GAUSSIAN
 - (C) CHARMM
 - (D) QUANTA
21. 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
22. Romberg integration is based on :
- (A) Richardson extrapolation of the Trapezoidal rule
 - (B) Bisection
 - (C) Gaussian elimination
 - (D) Taylor series only
23. Newton-Cotes formulas approximate the integral of a function using :
- (A) Tangent lines
 - (B) Polynomials
 - (C) Logarithms
 - (D) Sine waves
24. 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
25. 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
26. 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

27. Hermite interpolation requires knowledge of both function values and :
- (A) Second derivatives
 - (B) Integration constants
 - (C) First derivatives (slopes)
 - (D) Eigenvalues
28. 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
29. 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
30. 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
31. 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
32. An eigenvalue of a matrix A satisfies the equation :
- (A) $\det(A - \lambda I) = 0$
 - (B) $A\lambda = I$
 - (C) $\det(A) = \lambda$
 - (D) $A + \lambda I = 0$
33. The Householder method reduces a symmetric matrix to :
- (A) Diagonal form
 - (B) Identity form
 - (C) Tridiagonal form
 - (D) Triangular form
34. 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

35. Jacobi's method is used for finding eigenvalues of :
- (A) Any square matrix
 - (B) Singular matrices
 - (C) Only 2×2 matrices
 - (D) Symmetric matrices
36. 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
37. The Gauss-Jordan method results in the matrix becoming :
- (A) Upper triangular
 - (B) Lower triangular
 - (C) Reduced row echelon form (Identity)
 - (D) Singular
38. 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
39. The Gauss-Seidel method is an example of :
- (A) A direct method
 - (B) A recursive method
 - (C) An iterative method
 - (D) A symbolic method
40. 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
41. 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
42. The Regula-Falsi method is also known as :
- (A) Method of tangents
 - (B) Method of false position
 - (C) Interval halving
 - (D) Steepest descent

43. 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
44. What is the rate of convergence for the Newton-Raphson method ?
- (A) Linear
 - (B) Cubic
 - (C) Quadratic
 - (D) Logarithmic
45. 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
46. Which C operator is used to access the memory address of a variable ?
- (A) *
 - (B) ->
 - (C) &
 - (D) .
47. 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
48. 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
49. In Fortran, which statement is used to define a custom data type ?
- (A) struct
 - (B) record
 - (C) class
 - (D) type
50. Which feature in C allows a function to call itself ?
- (A) Iteration
 - (B) Recursion
 - (C) Inline expansion
 - (D) Nesting

51. Internet search results are ranked using :
- (A) Algorithms (like PageRank)
 - (B) Human voting
 - (C) Alphabetical order
 - (D) Random selection
52. The Schrödinger equation is a :
- (A) Linear algebraic equation
 - (B) Partial differential equation
 - (C) Quadratic equation
 - (D) Integral equation
53. Double precision in Fortran/C provides approximately :
- (A) 7 decimal digits
 - (B) 30 decimal digits
 - (C) 15-16 decimal digits
 - (D) 2 decimal digits
54. Ill-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
55. Searching scientific literature on the internet often uses :
- (A) Boolean operators (AND, OR, NOT)
 - (B) Only emojis
 - (C) Facebook
 - (D) Fortran
56. 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
57. Gauss-Jordan elimination is used to find the :
- (A) Inverse of a matrix
 - (B) Root of an equation
 - (C) Derivative
 - (D) Integral
58. Lagrange polynomials do not require :
- (A) Function values
 - (B) Equally spaced intervals
 - (C) Variable x
 - (D) A computer
59. Which is a 'Predictor-Corrector' method ?
- (A) Bisection
 - (B) Jacobi Method
 - (C) Gaussian Elimination
 - (D) Milne's Method

60. 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
61. A firewall in networking is used for :
- (A) Monitoring temperature
 - (B) Speeding up the mouse
 - (C) Security/Filtering unauthorized access
 - (D) Deleting spam
62. Ab initio methods solve the :
- (A) Electronic Schrödinger Equation
 - (B) Ideal Gas Equation
 - (C) Stock Market Equation
 - (D) Maxwell's Equations
63. The error in the Trapezoidal rule is of the order :
- (A) $O(h)$
 - (B) $O(h^2)$
 - (C) $O(h^4)$
 - (D) $O(1)$
64. Numerical integration is also called :
- (A) Numerical Quadrature
 - (B) Numerical Rooting
 - (C) Numerical Solving
 - (D) Numerical Factoring
65. 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
66. 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
67. Matrix ill-conditioning is checked using the :
- (A) Trace
 - (B) Condition Number
 - (C) Rank
 - (D) Size
68. 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

69. In C, a 'pointer' stores :
- (A) An integer value
 - (B) A memory address
 - (C) A character
 - (D) A floating point number
70. 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
71. 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
72. Structure-Activity Relationship (SAR) helps in :
- (A) Synthesis of chemicals
 - (B) Understanding how structural features affect biological response
 - (C) Naming molecules
 - (D) Measuring density
73. 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
74. '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
75. 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

76. 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
77. Central difference formula for differentiation is more accurate than :
- (A) Backward difference
 - (B) Forward difference
 - (C) Both (A) and (B)
 - (D) Neither
78. Matrix diagonalization of the Hamiltonian matrix gives :
- (A) Atomic coordinates
 - (B) Dipole moments
 - (C) Bond lengths
 - (D) Energy eigenvalues
79. What is the limit of ' h ' in the definition of a derivative ?
- (A) $h \rightarrow 1$
 - (B) $h \rightarrow \infty$
 - (C) $h \rightarrow 0$
 - (D) $h \rightarrow -1$
80. Ab initio packages like GAMESS are often written in :
- (A) HTML
 - (B) FORTRAN/C++
 - (C) Python only
 - (D) Java
81. The 'Hermite' interpolation polynomial matches both :
- (A) Function values and slopes
 - (B) Function values and integrals
 - (C) Slopes and curvature
 - (D) Value sat infinity
82. Convergence in Gauss-Seidel is faster if the matrix is :
- (A) Small
 - (B) Diagonally dominant
 - (C) Singular
 - (D) Symmetric only
83. 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

84. Which is NOT a valid molecular docking software ?
- (A) AutoDock
 - (B) GOLD
 - (C) Photoshop
 - (D) Glide
85. 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
86. A Fortran 'MODULE' is used for :
- (A) Deleting files
 - (B) Encapsulating data and subroutines
 - (C) Printing text
 - (D) Calculating square roots
87. The C library function 'pow(x , y)' is found in :
- (A) <stdio.h>
 - (B) <conio.h>
 - (C) <stdlib.h>
 - (D) <math.h>
88. The 'Hartree-Fock' method is a :
- (A) Semi-empirical method
 - (B) Ab initio method
 - (C) Molecular mechanics method
 - (D) Statistical averaging
89. Numerical differentiation using forward difference is :
- (A) First-order accurate
 - (B) Second-order accurate
 - (C) Fourth-order accurate
 - (D) Perfectly accurate
90. In a networking context, DNS stands for :
- (A) Data Network System
 - (B) Digital Node Server
 - (C) Domain Name System
 - (D) Direct Network Search
91. The 'Polynomial Wiggle' can be reduced by using :
- (A) Higher degree polynomials
 - (B) Spline interpolation (piecewise polynomials)
 - (C) Bisection
 - (D) Gaussian elimination
92. Which semi-empirical method is part of MOPAC ?
- (A) B3LYP
 - (B) CCSD(T)
 - (C) MP2
 - (D) AM1 or PM6

93. Gaussian 09 or 16 output files usually have the extension :
- (A) .exe
 - (B) .log or .out
 - (C) .png
 - (D) .mp3
94. The 'pivoting' strategy in Gaussian Elimination helps minimize :
- (A) Round
 - (B) Offerrors Logical
 - (C) Errors
 - (D) Memory usage
95. In C, '++i' is known as :
- (A) Post-increment
 - (B) Pre-increment
 - (C) Addition
 - (D) Pointer
96. Which method is 'self-starting' for solving ODEs ?
- (A) Adams-Bashforth
 - (B) Taylor series expansion beyond first term
 - (C) Predictor-Corrector
 - (D) Runge-Kutta
97. 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
98. The 'Newton-Cotes' formulas are used for :
- (A) Finding roots
 - (B) Numerical integration
 - (C) Sorting arrays
 - (D) Finding eigenvalues
99. 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
100. 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

(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 छँटना 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।