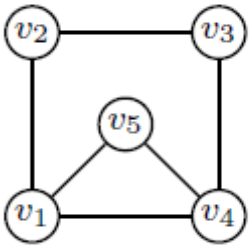
Course Director: MIHAI V. PUTZ **STUDENT NAME:**
Guest Lecturer: OTTORINO ORI
DATE:
GRADE (max=10p):

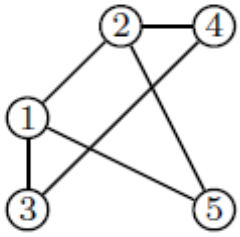
TEST
INTRODUCTION TO TOPOLOGICAL CHEMISTRY - NANO CHEMISTRY

START: 1p.

T1 (0.5p). Consider a unit cell with n_0 atoms. The cubic structure with L x L x L = L^3 total cells has then N = n_0 L^3 atoms. Being $Y=N^{1/3}$ express Y as a function of space dimension (d).

T2 (1p). Consider the following 2 isomorphic graphs and select the vertices correspondence evidencing the isomorphism.

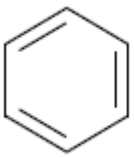




A(...) B(...) C(...)

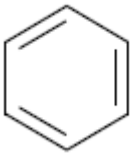
A(...)	B(...)	C(...)
v1 → 1, v2 → 3, v3 → 2, v4 → 5, v5 → 4	v1 → 1, v2 → 3, v3 → 4, v4 → 2, v5 → 5	v1 → 1, v2 → 3, v3 → 4, v4 → 2, v5 → 1

T3 (1p). After numbering 1,2,…6 the atoms of the benzene ring determine its 6x6 adjacency matrix A



$$A = \begin{pmatrix} 0 & \cdots \\ \vdots & \ddots & \vdots \\ \cdots & 0 \end{pmatrix}$$

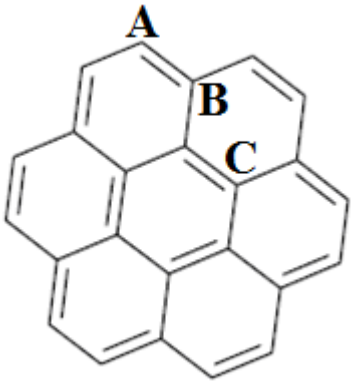
T4 (1p). After numbering 1,2,…6 the atoms of the benzene ring fill the distance matrix D and demonstrate that its Wiener number is equal to 27.



$$D = \begin{pmatrix} 0 & \cdots \\ \vdots & \ddots & \vdots \\ \cdots & 0 \end{pmatrix}$$

Suggestion: W(N)=6*w1

T5 (1p). Which is, topologically, the most stable atomic position in the Coronene molecule?



A(...) B(...) C(...)

T6 (1p). Indicating with wA, wB, wC the contribution to the Wiener index coming from atoms A,B,C above, which formula expresses correctly the Wiener number of this 24 atoms PAH?
NO CALCULATION REQUIRED ☺ JUST SYMMETRY CONSIDERATIONS

A(...) W= 12wA+ 6wB+6wC
B(...) W= 6wA+12wB+6wC
C(...) W= 6wA+ 6wB+6wC

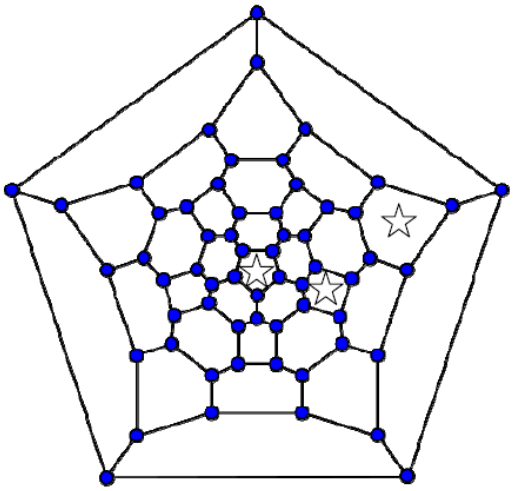
Suggestion:
use W(N)=nA*wA+ nB*wB+ nC*wC where nA is the number of atoms equivalent to A (A included) etc being N=nA + nB + nC

E7 (1p). Coronene molecule has 3 independent sites A,B,C with relative population n_A =12, n_B =n_C =6.

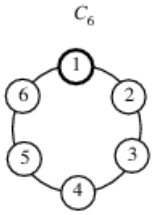
Which ^{13}C-NMR resonance pattern will then produce?

A(…) 3 lines with equal intensity
B(…) 3 lines with relative intensity 1,1,2
C(…) 3 lines with relative intensity 1,2,3

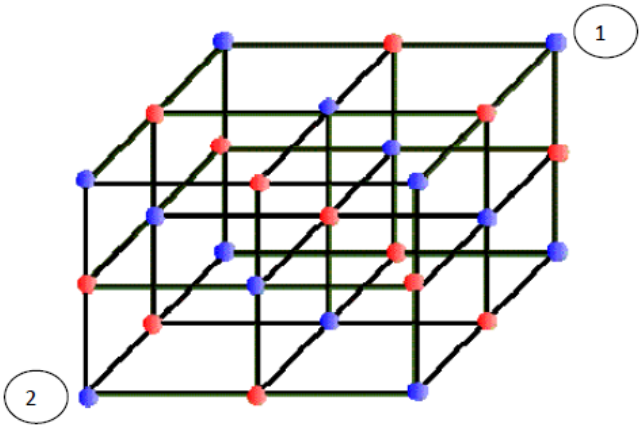
E8 (0.5p). Mark with a pencil the **12 pentagons** in the C_{60} planar graph. Some are already marked with a star…..



T9 (0.5). Having the closed linear graph with **EVEN NUMBER OF NODES** the Wiener index given by the following formula, $W(N)=N^3/8$, may you use it derive the Wiener index W=27 for the benzene ring?



T10 (0.5p). Indicate the maximum distance M we have in the graph connecting the opposite nodes 1 and 2



A(…) M=5 B(…) M=4 C(…) M=6

T11 (1p). Stars locate 2 sets of 4 faces 5|6|5|6 suitable for STONE-WALES rotations (in left figure). Mark with a pencil other possible quadruplets suitable for STONE-WALES rotations (in right figure).