

OLLSCOIL NA hÉIREANN, GAILLIMH  
NATIONAL UNIVERSITY OF IRELAND, GALWAY

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SUMMER EXAMINATIONS 2003

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Second Year Mathematics

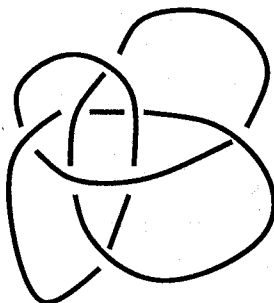
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**MA207 - Mathematics for Molecular Science.**

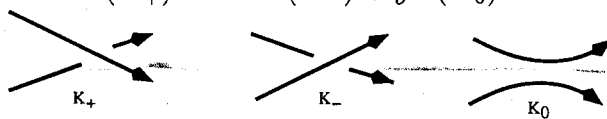
Dr Dave Johnson  
Professor T. Hurley  
Dr J. Burns  
Dr G. Ellis

Time allowed: *two* hours  
Attempt *three* questions

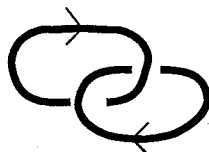
1. (a) Show that the following knot is 3-colourable, and explain how this proves that the knot isn't trivial.



- (b) Use the relation  $xP(K_+) + x^{-1}P(K_-) + yP(K_0) = 0$

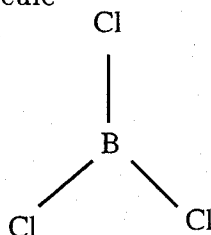


to compute the HOMFLY polynomial of the following link.



- (c) Define the linking number of a knot and explain how it is used to measure supercoiling in DNA.

2. (a) The boron trichloride molecule

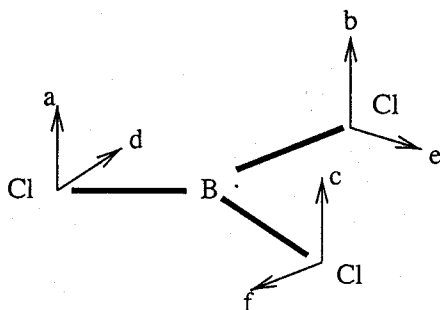


has point group  $D_{3h}$  whose character table is as follows.

$D_{3h}$	$E$	$2C_3$	$3C_2$	$\sigma_h$	$2S_3$	$3\sigma_v$	
$A'_1$	1	1	1	1	1	1	$x^2 + y^2, z^2$
$A'_2$	1	1	-1	1	1	-1	
$E'$	2	-1	0	2	-1	0	$(x, y) \quad (x^2 - y^2, xy)$
$A''_1$	1	1	1	-1	-1	-1	
$A''_2$	1	1	-1	-1	-1	1	$z$
$E''$	2	-1	0	-2	1	0	$(xz, yz)$

Determine the character  $\chi$  of  $D_{3h}$  generated by the three B-Cl bonds. Then express  $\chi$  as a sum of irreducible characters. What atomic orbitals might be used to construct a set of three  $\sigma$ -orbitals with lobes directed towards the chlorine atoms in  $BCl_3$ ?

- (b) Determine the character  $\chi'$  of  $D_{3h}$  generated by the six unit vectors  $a, \dots, f$  indicated below. (Vectors  $a$  and  $d$  are mutually perpendicular, and are also perpendicular to the B-Cl bond. The same is true for the pair  $b, e$  and the pair  $c, f$ .)



3. (a) Define the adjacency operator  $A$  on complex valued functions of a graph  $G$ . Prove that in the case of the Cayley graph  $X(\mathbb{Z}_n, \pm 1)$  the adjacency operator is a convolution operator. Hence by taking the discrete Fourier transform, prove that the spectrum of  $A$  is given by

$$\text{spec}(A) = \{2 \cos(2\pi a/n) | a = 0, 1, \dots, n-1\}.$$

- (b) Use part (a) to compute the rest mass energy  $E = \frac{2}{n} \sum \lambda$ , (where the sum is over the top  $n/2$  eigenvalues of  $A$ ), for benzene and cyclobutadiene. Explain the significance of your answers.

(P.T.O.)

4. (a) Let  $\delta_{\pm 1} : X(\mathbb{Z}_5, \pm 1) \rightarrow \mathbb{C}$  be the function which takes the value 1 at  $\pm 1$  and is zero otherwise, and let  $f(b) = b$ ,  $b \in \mathbb{Z}_n$ . Calculate the following, where  $\mathcal{F}$  denotes the discrete Fourier transform:

(i)  $\mathcal{F}f$ , and  $\mathcal{F}\delta_{\pm 1}$

(ii)  $\delta_{\pm 1} * f$ .

- (b) A particle moves at random with equal probability  $1/2$  to an adjacent vertex of the Cayley graph  $X(\mathbb{Z}_n, \pm 1)$  at discrete times  $j \in \mathbb{N}$ . Let  $u(b, j)$  denote the probability that the particle is at vertex  $b \in \mathbb{Z}_n$  at time  $j$ . Given that the particle starts at vertex 0 at time  $t = 0$ , prove that

$$u(b, j) = \frac{1}{n} \sum_{a \in \mathbb{Z}_n} (\cos(2\pi a/n))^j \exp(2\pi i ab/n).$$