

UNIVERSIDADE FEDERAL DE OURO PRETO
INSTITUTO DE CIÊNCIAS EXATAS E BIOLÓGICAS
DEPARTAMENTO DE MATEMÁTICA

Sexta Lista de Exercícios de Cálculo Diferencial e Integral III - MTM124
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05 de Fevereiro de 2016

- (1) Esboce a curva representada pelas equações paramétricas dadas, incluindo sua orientação; e determine sua equação cartesiana.

(a) $x(t) = 1 + t; y(t) = 1 - t$

(b) $x(t) = -1 + 2t, y(t) = 2 + 4t$

(c) $x(t) = 1 - t^2; y(t) = 2 + t^2$

(d) $x(t) = t + t^{-1}; y(t) = t - t^{-1}$
 [dica: Eleve ao quadrado e subtraia.]

(e) $x(t) = 3 \cos t; y(t) = 2 \sin t$

(f) $x(t) = 1 + t^2; y(t) = 3 - t$

(g) $x(t) = \sin t; y(t) = -3 + 2 \cos t$

(h) $x(t) = \sec t; y(t) = \tan t$

(i) $x(t) = t^3; y(t) = 1 - t^2$

(j) $x(t) = \sin t; y(t) = \cos 2t$

- (2) Sabendo que a função vetorial

$$\mathbf{r}(t) = P + t\vec{v}$$

com $t \in \mathbb{R}$ descreve a reta que passa pelo ponto P paralela ao vetor \vec{v} , se $P = (2, 5)$ e $\vec{v} = (-1, 1)$, esboce o gráfico.

- (3) Sejam $P = (1, 1)$ e $Q = (4, 2)$. (a) Faça o gráfico de $r(t) = tQ + (1 - t)P$ com $t \in [0, 1]$. (b) Verifique que as equações paramétricas do segmento de reta entre P e Q são $x(t) = 3t + 1; y(t) = t + 1; t \in [0, 1]$.

- (4) Encontre uma representação paramétrica para uma circunferência de centro em (h, k) e raio $a > 0$.

- (5) Calcular a derivada dy/dx das seguintes funções dadas na forma paramétrica. Para quais valores de t a derivada está definida? Trace os gráficos das funções.

(a) $\begin{cases} x(t) = t^2, \\ y(t) = t^3, \end{cases} \quad t \in (0, +\infty)$

(b) $\begin{cases} x(t) = \cos 2t, \\ y(t) = \sin 2t, \end{cases} \quad t \in [0, \pi/2]$

(c) $\begin{cases} x(t) = 3 \cos t, \\ y(t) = 4 \sin t, \end{cases} \quad t \in [\pi, 2\pi]$

(d) $\begin{cases} x(t) = \cos^3 t, \\ y(t) = \sin^3 t, \end{cases} \quad t \in (-\pi/2, 0)$

(e) $\begin{cases} x(t) = 2t - 1, \\ y(t) = t^3 + 5, \end{cases} \quad -\infty < t < +\infty$

(f) $\begin{cases} x(t) = 8 \cos^3 t, \\ y(t) = 8 \sin^3 t, \end{cases} \quad t \in [0, \pi]$

- (6) Chama-se *ciclóide* a curva gerada pelo caminho percorrido por um ponto P fixo em uma circunferência de raio a , quando esta circunferência gira, sem deslizar, sobre uma linha reta (considere o eixo- x). Encontre as equações paramétricas da ciclóide. [Dica: mostre que, por translação de eixos, $x = at + x'$ e $y = a + y'$ e obtenha x' e y' em função de t . Ver figura.]

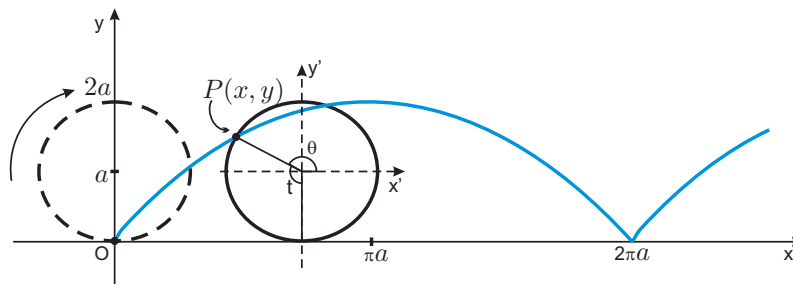


FIGURA 1. Ciclóide

- (7) ‡ Para um caminho $\gamma(t)$ para $t \in [a, b]$ dado, a *função comprimento de arco* a partir de $\gamma(a)$, denotada por $s(t)$, é definida por

$$s(t) = \int_a^t \|\gamma'(t)\| dt \quad (0.1)$$

e fornece, para cada $t \in [a, b]$, a distância sobre γ entre $\gamma(a)$ e $\gamma(t)$. Encontre a função comprimento de arco a partir de $\gamma(0)$ para as curvas $\alpha(t) = (\cosh t, \sinh t, t)$, $\beta(t) = (\cos t, \sin t, t)$, e $\gamma(t) = (\cos(t/\sqrt{2}), \sin(t/\sqrt{2}), t/\sqrt{2})$.

- (8) ‡ Seja $\gamma : [a, b] \rightarrow \mathbb{R}^3$, um caminho dado e seja $s = \alpha(t)$ uma nova variável, onde α é uma função real de classe C^1 estritamente crescente, definida no intervalo $[a, b]$. Da monotonicidade de α , para cada $s \in [\alpha(a), \alpha(b)]$ existe um único t com $\alpha(t) = s$. Defina a função $\Gamma : [\alpha(a), \alpha(b)] \rightarrow \mathbb{R}^3$ por $\Gamma(s) = \gamma(t)$. (a) Convença-se de que os traços das curvas $\gamma(t)$ e $\Gamma(s)$ é o mesmo. (b) Prove que γ e Γ tem o mesmo comprimento de arco. (c) Seja $s(t)$ como em (0.1). Defina $\tilde{\gamma}$ como acima por $\tilde{\gamma}(s) = \gamma(t)$. Mostre que

$$\left\| \frac{d}{ds} \tilde{\gamma}(s) \right\| = 1.$$

(O caminho $s \mapsto \tilde{\gamma}(s)$ é chamado *reparametrização pelo comprimento de arco* de γ .)

- (9) ‡ Seja $\sigma : [a, b] \rightarrow \mathbb{R}^3$ uma curva suave (derivatives of all orders exist). Assuma que $\sigma'(t) \neq 0$ para todo t . O vetor $T(t) = \sigma'(t)/\|\sigma'(t)\|$ é tangente a σ no ponto $\sigma(t)$ e como $\|T(t)\| = 1$ ele é chamado de vetor tangente unitário. Use a regra do produto (escalar) para derivar $T'(t) \cdot T(t) = 1$ e mostrar que $T'(t) \cdot T(t) = 0$.

- (10) ‡ Um caminho σ está parametrizado pelo comprimento de arco se $\|\sigma'(s)\| = 1$. (a) Para um caminho parametrizado pelo comprimento de arco em $[a, b]$, mostre que o comprimento de σ é $L(\sigma) = b - a$. (b) A *curvatura* de uma curva σ em um ponto $\sigma(s)$ é definida por $\kappa = \|T'(s)\|$ quando o caminho está parametrizado pelo comprimento de arco. Mostre que $\kappa = \|\sigma''(s)\|$. (c) Se σ é dado em termos de algum outro parâmetro t e $\sigma(t)$ nunca é zero, mostre que

$$\kappa = \|\sigma'(t) \times \sigma''(t)\| / \|\sigma'(t)\|^3.$$

- (d) Calcule a curvatura da hélice $\gamma(t) = (1/\sqrt{2})(\cos t, \sin t, t)$.

- (11) Calcule o comprimento das curvas dadas pelas seguintes funções vetoriais:

(a) Hélice circular: $\mathbf{r}(t) = 2 \cos t \mathbf{i} + 2 \sin t \mathbf{j} + 6t \mathbf{k}$; de $(2, 0, 0)$ a $(2, 0, 24\pi)$.

(b) Catenária: $\mathbf{r}(t) = t \mathbf{i} + \cosh t \mathbf{j}$ de $t = 0$ a $t = 1$.

(c) Hipociclóide: $\mathbf{r}(t) = a \cos^3 t \mathbf{i} + a \sin^3 t \mathbf{j}$; comprimento total

- (12) Encontre a curvatura em cada ponto P . Esboce (ou plote) a curva.

(a) $y = 2 - x^3$; $P = (1, 1)$; (b) $y = e^{x^2}$; $P = (0, 1)$;

(c) $y = \cos(2x)$; $P = (0, 1)$; (d) $\begin{cases} x(t) = t - 1, \\ y(t) = \sqrt{t}, \end{cases} P = (3, 2)$;

(e) $\begin{cases} x(t) = t - t^2, \\ y(t) = 1 - t^3, \end{cases} P = (0, 1)$; (f) $\mathbf{r}(t) = 2 \sin(t) \mathbf{i} + 3 \cos(t) \mathbf{j}$; $P = (1, 3\sqrt{3}/2)$.

- (13) Se a curvatura κ em um ponto P de uma curva Γ é diferente de zero, ao número $\rho = 1/\kappa$ chamamos de *Raio de Curvatura* em P e ao círculo de raio ρ cujo centro está no lado côncavo de C e que compartilha a reta tangente em P com a curva C chamamos de *Círculo de Curvatura* (ou *Círculo Osculador*) em P . Seu centro recebe o nome de *Centro de Curvatura* em P . Para as curvas a seguir, encontre o raio de curvatura em P , o círculo de curvatura em P e esboce a curva e o círculo de curvatura em P . (a) $y = \sin x$; $P = (\pi/2, 1)$ (b) $y = e^x$; $P = (0, 1)$.

- (14) Sendo $\mathbf{T}(s)$ e $\mathbf{N}(s)$ respectivamente os vetores tangente unitário e normal principal unitário a uma curva espacial C parametrizada pelo comprimento de arco s , dada pela função $\mathbf{r}(s)$. Definimos

o *Vetor Binormal unitário*, denotado por $\mathbf{B}(s)$, por

$$\mathbf{B}(s) = \mathbf{T}(s) \times \mathbf{N}(s). \quad (0.2)$$

Assim, o referencial ortonormal positivo $\{\mathbf{T}(s), \mathbf{N}(s), \mathbf{B}(s)\}$ é chamado de *Triedro de Frenet* de C em s .

(a) Mostre que $\mathbf{B}'(s) = \mathbf{T}(s) \times \mathbf{N}'(s)$ e conclua que $\mathbf{B}'(s)$ é ortogonal a $\mathbf{T}(s)$. [Dica: Derive (0.2), use a regra do produto vetorial e que $\mathbf{T}'(s) = \kappa(s) \times \mathbf{N}(s)$].

(b) Como $\|\mathbf{B}(s)\| = 1$, temos $\mathbf{B}(s) \cdot \mathbf{B}(s) = 1$. Derive esta expressão e obtenha $\mathbf{B}'(s) \cdot \mathbf{B}(s) = 0$ e conclua que $\mathbf{B}'(s)$ é ortogonal a $\mathbf{B}(s)$.

(c) Dos *itens* anteriores perceba que $\mathbf{B}'(s)$ é paralelo a $\mathbf{N}(s)$, isto é, $\mathbf{B}'(s)$ é igual ao produto de $\mathbf{N}(s)$ por um número real τ (que depende de s).

(d) Conclua que podemos definir,

$$\mathbf{B}'(s) = \tau(s)\mathbf{N}(s),$$

a *torção da curva C em s* .

(15) Sendo $\mathbf{T}(s), \mathbf{N}(s), \mathbf{B}(s)$ respectivamente os vetores tangente, normal e binormal a uma curva espacial C parametrizada pelo comprimento de arco s , dada pela função $\mathbf{r}(s)$ e sabendo que a torção $\tau(s)$ desta curva é dada pela expressão $\mathbf{B}'(s) = \tau(s)\mathbf{N}(s)$, prove que podemos calcular a torção utilizando a expressão $\tau(s) = \mathbf{N}(s) \cdot \mathbf{B}'(s)$. [Dica, use que $\mathbf{N} \cdot \mathbf{N} = 1$.]

(16) Sejam $y = x^4 - 12x^2$ e $y = \sinh(x)$. Alguma destas curvas admite algum ponto com curvatura zero? Que pontos são estes?

(17) (†) Encontre a curvatura em (x, y, z) da hélice elíptica

$$\mathbf{r}(t) = a \cos(t)\mathbf{i} + b \sin(t)\mathbf{j} + ct\mathbf{k},$$

onde a, b e c são constantes estritamente positivas.

(18) (*Ciclóide*) O caminho de um ponto fixo em uma roda de raio a que rola sem escorregar ou derrapar ao longo do eixo- x é dado por

$$\mathbf{r}(t) = (a \sin(\omega t) + \omega at)\mathbf{i} + (a \cos(\omega t) + a)\mathbf{j}.$$

Encontre a velocidade e a aceleração deste ponto no momento em que ele atinge o valor máximo no eixo- y .

(19) Se \mathbf{T} representa o vetor tangente unitário, \mathbf{N} o vetor normal unitário, s o parâmetro comprimento de arco, κ a curvatura e ν o módulo da velocidade de uma partícula P percorrendo uma curva dada por $\mathbf{r}(t)$; sabendo que $\mathbf{T}'(s) = \kappa\mathbf{N}(s)$ e $\nu = \|\mathbf{r}'(t)\| = ds/dt$, obtenha a expressão

$$\mathbf{r}''(t) = \frac{d^2s}{dt^2}\mathbf{T}(s) + \left(\frac{ds}{dt}\right)^2 \kappa\mathbf{N}(s),$$

ou equivalentemente

$$\mathbf{r}''(t) = \frac{d\nu}{dt}\mathbf{T}(s) + \nu^2\kappa\mathbf{N}(s), \quad (0.3)$$

derivando a equação $\mathbf{r}'(t) = \frac{ds}{dt}\mathbf{T}(s)$. [Dica: Use a regra da cadeia e a regra do produto, lembre-se $s = s(t)$]. A expressão (0.3) nos dá a aceleração $\mathbf{r}''(t)$ em termos de sua componente normal $d\nu/dt$ (taxa de variação do módulo da velocidade com respeito ao tempo) e tangencial $\nu^2\kappa$.

(20) (†) (*Jerk*) Atualmente, a terceira derivada $\mathcal{J}(t) = \mathbf{r}'''(t)$, em inglês conhecida como *Jerk*, é também de interesse em aplicações em engenharia (como em análise de mecanismos, estudo de conforto em veículos, cam design, entre outros). Mostre a partir de (0.3) que

$$\mathcal{J} = \left(\frac{d^2\nu}{dt^2} - \kappa^2\nu^3\right)\mathbf{T} + 3\kappa\nu\frac{d\nu}{dt}\mathbf{N} - \kappa\nu^3\mathbf{B},$$

onde \mathbf{v} é o vetor velocidade e \mathbf{B} é o vetor binormal.

- (21) Engrenagens, transmissões e outras construções de engenharia as vezes envolvem complicados caminhos (curvas) que são estudados através do uso de softwares gráficos. Para se ter uma ideia, plote os seguintes caminhos e encontre a velocidade, o módulo da velocidade, e a aceleração tangencial e normal.

(a) $\mathbf{r}(t) = (2 \cos t + \cos 2t)\mathbf{i} + (2 \sin t - \sin 2t)\mathbf{j}$ (Hipociclóide de Steiner)

(b) $\mathbf{r}(t) = (\cos t + \cos 2t)\mathbf{i} + (\sin t - \sin 2t)\mathbf{j}$

(c) $\mathbf{r}(t) = \cos(t)\mathbf{i} + \sin(2t)\mathbf{j} + \cos(2t)\mathbf{k}$

(d) $\mathbf{r}(t) = ct \cos(t)\mathbf{i} + ct \sin(t)\mathbf{j} + ct\mathbf{k}$

- (22) (*Velocidade angular*) Suponha que uma partícula P está girando em torno do eixo- z , numa trajetória circular de raio a em um plano paralelo ao plano- xy . Suponha que a variação $d\theta/dt$ é constante igual a ω . O vetor $\vec{\omega} = \omega\mathbf{k}$ (paralelo ao eixo- z com magnitude ω) é chamado de *velocidade angular* de P . Se $\mathbf{r}(t) = a \cos(\omega t)\mathbf{i} + a \sin(\omega t)\mathbf{j} + h\mathbf{k}$, mostre que $\vec{\omega} \times \mathbf{r}(t) = \mathbf{r}'(t)$.

- (23) (*Sol e Terra*) Encontre a aceleração da Terra girando em torno do Sol considerando que o movimento pode ser aproximado por uma órbita aproximadamente circular dada por

$$\mathbf{r}(t) = R \cos(\omega t)\mathbf{i} + R \sin(\omega t)\mathbf{j},$$

e que o módulo da velocidade é quase constante igual a $30\text{km}/\text{seg}$.

[Dica: $a = r'' = -R\omega^2 \cos(\omega t)\mathbf{i} - R\omega^2 \sin(\omega t)\mathbf{j}$.]

- (24) (*Terra e Lua*) Encontre a aceleração centrípeta $\mathbf{a} = -\omega^2\mathbf{r}$ da Lua girando em torno da Terra, assumindo que a órbita da Lua é um círculo de raio $3,85 \cdot 10^5$ quilômetros e o tempo para uma revolução completa é $27,3$ dias $= 2,36 \cdot 10^6$ segundos.

- (25) Faça o que se pede.

(a) Primeiro, mostre que um círculo de raio a tem curvatura $1/a$.

(b) Agora, calcule a curvatura da curva $\mathbf{r}(t) = \int_0^t \sin(\pi t^2/2) dt \mathbf{i} + \int_0^t \cos(\pi t^2/2) dt \mathbf{j}$.

- (26) Se C é uma curva com $\kappa > 0$, representada por $\mathbf{r}(t)$ onde t é um parâmetro qualquer, é possível obter a curvatura e a torção a partir das expressões

$$\kappa(t) = \frac{\|\mathbf{r}'(t) \times \mathbf{r}''(t)\|}{\|\mathbf{r}'(t)\|^3} \quad \text{e} \quad \tau(t) = \frac{(\mathbf{r}'(t) \times \mathbf{r}''(t)) \cdot \mathbf{r}'''(t)}{\|\mathbf{r}'(t) \times \mathbf{r}''(t)\|^2}.$$

Calcule a curvatura e a torção da curva $\mathbf{r}(t) = t\mathbf{i} + t^2\mathbf{j} + t^3\mathbf{k}$.

- (27) Mostre que a hélice $a \cos(t)\mathbf{i} + a \sin(t)\mathbf{j} + ct\mathbf{k}$ pode ser representada por $a \cos(s/K)\mathbf{i} + a \sin(s/K)\mathbf{j} + c(s/K)\mathbf{k}$, onde $K = \sqrt{a^2 + c^2}$ e s é o comprimento de arco. Mostre que a hélice tem curvatura $\kappa(t) = a/K^2$ e torção $\tau(t) = c/K^2$ constantes.

Fato interessante: A molécula de DNA tem a forma de duas hélices circulares.

- (28) Se u é uma função escalar, o *Laplaciano* de u , é definido como $\Delta u := \text{div}(\nabla u)$.

(a) Mostre que $\Delta u(x, y) = u_{xx} + u_{yy}$, (b) Se $u(x, y) = \ln \sqrt{x^2 + y^2}/2\pi$, calcule Δu .

- (29) (Identidades de Green) Faça o que se pede:

(a) Use o Teorema de Green na versão que foi vista em sala para provar a seguinte *Forma Vetorial do Teorema de Green*

$$\oint_{\partial D} \mathbf{F} \cdot \mathbf{n} ds = \iint_D \nabla \cdot \mathbf{F} dA,$$

onde $\mathbf{n} = (y'(t)\mathbf{i} - x'(t)\mathbf{j})/|r'(t)|$ é o vetor unitário, normal à curva, apontando para seu exterior.

(b) Use uma versão vetorial do Teorema de Green (a do exercício anterior) para provar a **Primeira Identidade de Green**

$$\iint_D f \Delta g dA = \oint_{\partial D} f(\nabla g) \cdot \mathbf{n} ds - \iint_D \nabla f \cdot \nabla g dA,$$

para funções f e g com derivadas suficientemente contínuas e uma região D com fronteira suficientemente suave. (Nota: A quantidade $\nabla g \cdot \mathbf{n}$ que aparece na segunda integral acima, é a derivada direcional de g na direção do vetor normal unitário \mathbf{n} , às vezes denotada por $\frac{\partial g}{\partial \mathbf{n}}$. Esta derivada é comumente chamada de *derivada normal* de g .)

(c) Sob as mesmas hipóteses, use a Primeira Identidade de Green para provar a **Segunda Identidade de Green**

$$\iint_D (f \Delta g - g \Delta f) dA = \oint_{\partial D} (f \nabla g - g \nabla f) \cdot \mathbf{n} ds.$$

- (30) Em Biologia Molecular, a expressão dupla hélice é utilizada para descrever a estrutura de ácidos nucleicos, como o DNA. A doutora **Rosalind Franklin** do *Wheatstone Physics Laboratory* do *King's College* de Londres, publicou em 1953 na revista *Nature* um importante artigo (que se encontra nas duas páginas seguintes, para seu deleite, mas de leitura opcional) onde se afirma que a estrutura do DNA tem a forma de duas hélices circulares de diâmetro igual a 20 angströms ($1\text{\AA} = 10^{-8} \text{cm}$) e que cada hélice em uma volta completa sobe 34\AA . Adicionalmente, sabe-se que que existem cerca de $2,9 \times 10^8$ voltas completas em uma molécula. Estima-se que o comprimento de cada Hélice circular pode chegar a 2m. Prove essa última afirmação.

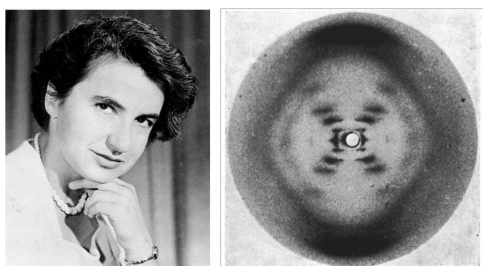


FIGURA 2. Doutora Rosalind Franklin e a famosa "Photo 51".

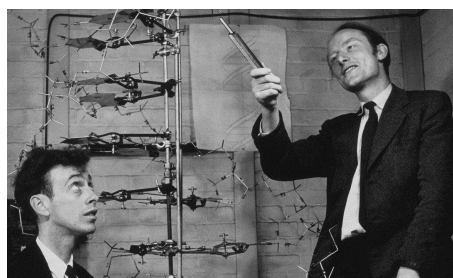


FIGURA 3. James Watson (esq.) e Francis Crick (dir.)

$$\begin{aligned} & R.1a.x + y = 2; 1b.2x - y = -4; 1c.x + y = 3; 1f.x - 1 = (y - 3)^2; 1h.x^2 - y^2 = 1; 1j.y = 1 - 2x^2; \\ & 4.x = h + a \cos t; y = k + a \sin t; 11b.\sinh 1; 26.\kappa(1) = \frac{1}{7}\sqrt{19/14}. \end{aligned}$$

Bom Estudo!

6ª Lista MTM124

We wish to thank Prof. J. T. Randall for encouragement; Profs. E. Chargaff, R. Signer, J. A. V. Butler and Drs. J. D. Watson, J. D. Smith, L. Hamilton, J. C. White and G. R. Wyatt for supplying material without which this work would have been impossible; also Drs. J. D. Watson and Mr. F. H. C. Crick for stimulation, and our colleagues R. E. Franklin, R. G. Gosling, G. L. Brown and W. E. Seeds for discussion. One of us (H. R. W.) wishes to acknowledge the award of a University of Wales Fellowship.

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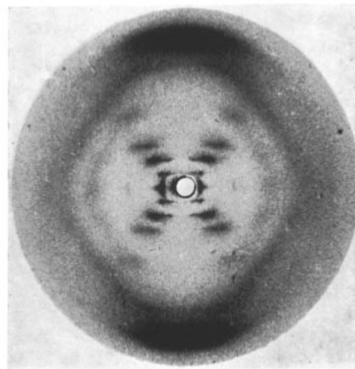
Molecular Configuration in Sodium Thymonucleate

SODIUM thymonucleate fibres give two distinct types of X-ray diagram. The first corresponds to a crystalline form, structure *A*, obtained at about 75 per cent relative humidity; a study of this is described in detail elsewhere¹. At higher humidities a different structure, structure *B*, showing a lower degree of order, appears and persists over a wide range of ambient humidity. The change from *A* to *B* is reversible. The water content of structure *B* fibres which undergo this reversible change may vary from 40-50 per cent to several hundred per cent of the dry weight. Moreover, some fibres never show structure *A*, and in these structure *B* can be obtained with an even lower water content.

The X-ray diagram of structure *B* (see photograph) shows in striking manner the features characteristic of helical structures, first worked out in this laboratory by Stokes (unpublished) and by Crick, Cochran and Vand². Stokes and Wilkins were the first to propose such structures for nucleic acid as a result of direct studies of nucleic acid fibres, although a helical structure had been previously suggested by Furberg (thesis, London, 1949) on the basis of X-ray studies of nucleosides and nucleotides.

While the X-ray evidence cannot, at present, be taken as direct proof that the structure is helical, other considerations discussed below make the existence of a helical structure highly probable.

Structure *B* is derived from the crystalline structure *A* when the sodium thymonucleate fibres take up quantities of water in excess of about 40 per cent of their weight. The change is accompanied by an increase of about 30 per cent in the length of the fibre, and by a substantial re-arrangement of the molecule. It therefore seems reasonable to suppose that in structure *B* the structural units of sodium thymonucleate (molecules or groups of molecules) are relatively free from the influence of neighbouring



Sodium deoxyribose nucleate from calf thymus. Structure *B*

molecules, each unit being shielded by a sheath of water. Each unit is then free to take up its least-energy configuration independently of its neighbours and, in view of the nature of the long-chain molecules involved, it is highly likely that the general form will be helical³. If we adopt the hypothesis of a helical structure, it is immediately possible, from the X-ray diagram of structure *B*, to make certain deductions as to the nature and dimensions of the helix.

The innermost maxima on the first, second, third and fifth layer lines lie approximately on straight lines radiating from the origin. For a smooth single-strand helix the structure factor on the *n*th layer line is given by:

$$F_n = J_n(2\pi rR) \exp i n(\psi + \frac{1}{2}\pi),$$

where $J_n(u)$ is the *n*th-order Bessel function of u , r is the radius of the helix, and R and ψ are the radial and azimuthal co-ordinates in reciprocal space²; this expression leads to an approximately linear array of intensity maxima of the type observed, corresponding to the first maxima in the functions J_1, J_2, J_3 , etc.

If, instead of a smooth helix, we consider a series of residues equally spaced along the helix, the transform in the general case treated by Crick, Cochran and Vand is more complicated. But if there is a whole number, m , of residues per turn, the form of the transform is as for a smooth helix with the addition, only, of the same pattern repeated with its origin at heights mc^* , $2mc^*$. . . etc. (c is the fibre-axis period).

In the present case the fibre-axis period is 34 Å. and the very strong reflexion at 3.4 Å. lies on the tenth layer line. Moreover, lines of maxima radiating from the 3.4-Å. reflexion as from the origin are visible on the fifth and lower layer lines, having a J_5 maximum coincident with that of the origin series on the fifth layer line. (The strong outer streaks which apparently radiate from the 3.4-Å. maximum are not, however, so easily explained.) This suggests strongly that there are exactly 10 residues per turn of the helix. If this is so, then from a measurement of R_n the position of the first maximum on the *n*th layer line (for $n \ll 5$), the radius of the helix, can be obtained. In the present instance, measurements of R_1, R_2, R_3 and R_4 all lead to values of r of about 10 Å.

Since this linear array of maxima is one of the strongest features of the X-ray diagram, we must conclude that a crystallographically important part of the molecule lies on a helix of this diameter. This can only be the phosphate groups or phosphorus atoms.

If ten phosphorus atoms lie on one turn of a helix of radius 10 Å., the distance between neighbouring phosphorus atoms in a molecule is 7.1 Å. This corresponds to the P . . . P distance in a fully extended molecule, and therefore provides a further indication that the phosphates lie on the outside of the structural unit.

Thus, our conclusions differ from those of Pauling and Corey¹, who proposed for the nucleic acids a helical structure in which the phosphate groups form a dense core.

We must now consider briefly the equatorial reflexions. For a single helix the series of equatorial maxima should correspond to the maxima in $J_0(2\pi rR)$. The maxima on our photograph do not, however, fit this function for the value of r deduced above. There is a very strong reflexion at about 24 Å. and then only a faint sharp reflexion at 9.0 Å. and two diffuse bands around 5.5 Å. and 4.0 Å. This lack of agreement is, however, to be expected, for we know that the helix so far considered can only be the most important member of a series of coaxial helices of different radii; the non-phosphate parts of the molecule will lie on inner co-axial helices, and it can be shown that, whereas these will not appreciably influence the innermost maxima on the layer lines, they may have the effect of destroying or shifting both the equatorial maxima and the outer maxima on other layer lines.

Thus, if the structure is helical, we find that the phosphate groups or phosphorus atoms lie on a helix of diameter about 20 Å., and the sugar and base groups must accordingly be turned inwards towards the helical axis.

Considerations of density show, however, that a cylindrical repeat unit of height 34 Å. and diameter 20 Å. must contain many more than ten nucleotides.

Since structure *B* often exists in fibres with low water content, it seems that the density of the helical unit cannot differ greatly from that of dry sodium thymonucleate, 1.63 gm./cm.³^{1,2}, the water in fibres of high water-content being situated outside the structural unit. On this basis we find that a cylinder of radius 10 Å. and height 34 Å. would contain thirty-two nucleotides. However, there might possibly be some slight inter-penetration of the cylindrical units in the dry state making their effective radius rather less. It is therefore difficult to decide, on the basis of density measurements alone, whether one repeating unit contains ten nucleotides on each of two or on each of three co-axial molecules. (If the effective radius were 8 Å. the cylinder would contain twenty nucleotides.) Two other arguments, however, make it highly probable that there are only two co-axial molecules.

First, a study of the Patterson function of structure *A*, using superposition methods, has indicated³ that there are only two chains passing through a primitive unit cell in this structure. Since the $A \rightleftharpoons B$ transformation is readily reversible, it seems very unlikely that the molecules would be grouped in threes in structure *B*. Secondly, from measurements on the X-ray diagram of structure *B* it can readily be shown that, whether the number of chains per unit is two or three, the chains are not equally spaced along the

fibre axis. For example, three equally spaced chains would mean that the n th layer line depended on J_{3n} , and would lead to a helix of diameter about 60 Å. This is many times larger than the primitive unit cell in structure *A*, and absurdly large in relation to the dimensions of nucleotides. Three unequally spaced chains, on the other hand, would be crystallographically non-equivalent, and this, again, seems unlikely. It therefore seems probable that there are only two co-axial molecules and that these are unequally spaced along the fibre axis.

Thus, while we do not attempt to offer a complete interpretation of the fibre-diagram of structure *B*, we may state the following conclusions. The structure is probably helical. The phosphate groups lie on the outside of the structural unit, on a helix of diameter about 20 Å. The structural unit probably consists of two co-axial molecules which are not equally spaced along the fibre axis, their mutual displacement being such as to account for the variation of observed intensities of the innermost maxima on the layer lines; if one molecule is displaced from the other by about three-eighths of the fibre-axis period, this would account for the absence of the fourth layer line maxima and the weakness of the sixth. Thus our general ideas are not inconsistent with the model proposed by Watson and Crick in the preceding communication.

The conclusion that the phosphate groups lie on the outside of the structural unit has been reached previously by quite other reasoning¹. Two principal lines of argument were invoked. The first derives from the work of Gulland and his collaborators⁴, who showed that even in aqueous solution the $-\text{CO}$ and $-\text{NH}_2$ groups of the bases are inaccessible and cannot be titrated, whereas the phosphate groups are fully accessible. The second is based on our own observations¹ on the way in which the structural units in structures *A* and *B* are progressively separated by an excess of water, the process being a continuous one which leads to the formation first of a gel and ultimately to a solution. The hygroscopic part of the molecule may be presumed to lie in the phosphate groups $((\text{C}_2\text{H}_4\text{O})_2\text{PO}_2\text{Na}$ and $(\text{C}_2\text{H}_4\text{O})_2\text{PO}_2\text{Na}$ are highly hygroscopic⁵), and the simplest explanation of the above process is that these groups lie on the outside of the structural units. Moreover, the ready availability of the phosphate groups for interaction with proteins can most easily be explained in this way.

We are grateful to Prof. J. T. Randall for his interest and to Drs. F. H. C. Crick, A. R. Stokes and M. H. F. Wilkins for discussion. One of us (R. E. F.) acknowledges the award of a Turner and Newall Fellowship.

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FIGURA 4. Franklin's article.

equipment, and to Dr. G. E. R. Deacon and the captain and officers of R.R.S. *Discovery II* for their part in making the observations.

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MOLECULAR STRUCTURE OF NUCLEIC ACIDS

A Structure for Deoxyribose Nucleic Acid

WE wish to suggest a structure for the salt of deoxyribose nucleic acid (D.N.A.). This structure has novel features which are of considerable biological interest.

A structure for nucleic acid has already been proposed by Pauling and Corey¹. They kindly made their manuscript available to us in advance of publication. Their model consists of three intertwined chains, with the phosphates near the fibre axis, and the bases on the outside. In our opinion, this structure is unsatisfactory for two reasons: (1) We believe that the material which gives the X-ray diagrams is the salt, not the free acid. Without the acidic hydrogen atoms it is not clear what forces would hold the structure together, especially as the negatively charged phosphates near the axis will repel each other. (2) Some of the van der Waals distances appear to be too small.

Another three-chain structure has also been suggested by Fraser (in the press). In his model the phosphates are on the outside and the bases on the inside, linked together by hydrogen bonds. This structure as described is rather ill-defined, and for this reason we shall not comment on it.

We wish to put forward a radically different structure for the salt of deoxyribose nucleic acid. This structure has two helical chains each coiled round the same axis (see diagram). We have made the usual chemical assumptions, namely, that each chain consists of phosphate diester groups joining β -D-deoxy-ribofuranose residues with 3',5' linkages. The two chains (but not their bases) are related by a dyad perpendicular to the fibre axis. Both chains follow right-handed helices, but owing to the dyad the sequences of the atoms in the two chains run in opposite directions. Each chain loosely resembles Furberg's² model No. 1; that is, the bases are on the inside of the helix and the phosphates on the outside. The configuration of the sugar and the atoms near it is close to Furberg's 'standard configuration', the sugar being roughly perpendicular to the attached base. There



This figure is purely diagrammatic. The two ribbons symbolize the two phosphate-sugar chains, and the horizontal rods the pairs of bases holding the chains together. The vertical line marks the fibre axis.

is a residue on each chain every 3.4 Å. in the z-direction. We have assumed an angle of 36° between adjacent residues in the same chain, so that the structure repeats after 10 residues on each chain, that is, after 34 Å. The distance of a phosphorus atom from the fibre axis is 10 Å. As the phosphates are on the outside, cations have easy access to them.

The structure is an open one, and its water content is rather high. At lower water contents we would expect the bases to tilt so that the structure could become more compact.

The novel feature of the structure is the manner in which the two chains are held together by the purine and pyrimidine bases. The planes of the bases are perpendicular to the fibre axis. They are joined together in pairs, a single base from one chain being hydrogen-bonded to a single base from the other chain, so that the two lie side by side with identical z-co-ordinates. One of the pair must be a purine and the other a pyrimidine for bonding to occur. The hydrogen bonds are made as follows: purine position 1 to pyrimidine position 1; purine position 6 to pyrimidine position 6.

If it is assumed that the bases only occur in the structure in the most plausible tautomeric forms (that is, with the keto rather than the enol configurations) it is found that only specific pairs of bases can bond together. These pairs are: adenine (purine) with thymine (pyrimidine), and guanine (purine) with cytosine (pyrimidine).

In other words, if an adenine forms one member of a pair, on either chain, then on these assumptions the other member must be thymine; similarly for guanine and cytosine. The sequence of bases on a single chain does not appear to be restricted in any way. However, if only specific pairs of bases can be formed, it follows that if the sequence of bases on one chain is given, then the sequence on the other chain is automatically determined.

It has been found experimentally^{3,4} that the ratio of the amounts of adenine to thymine, and the ratio of guanine to cytosine, are always very close to unity for deoxyribose nucleic acid.

It is probably impossible to build this structure with a ribose sugar in place of the deoxyribose, as the extra oxygen atom would make too close a van der Waals contact.

The previously published X-ray data^{5,6} on deoxyribose nucleic acid are insufficient for a rigorous test of our structure. So far as we can tell, it is roughly compatible with the experimental data, but it must be regarded as unproved until it has been checked against more exact results. Some of these are given in the following communications. We were not aware of the details of the results presented there when we devised our structure, which rests mainly though not entirely on published experimental data and stereochemical arguments.

It has not escaped our notice that the specific pairing we have postulated immediately suggests a possible copying mechanism for the genetic material.

Full details of the structure, including the conditions assumed in building it, together with a set of co-ordinates for the atoms, will be published elsewhere.

We are much indebted to Dr. Jerry Donohue for constant advice and criticism, especially on interatomic distances. We have also been stimulated by a knowledge of the general nature of the unpublished experimental results and ideas of Dr. M. H. F. Wilkins, Dr. R. E. Franklin and their co-workers at

King's College, London. One of us (J. D. W.) has been aided by a fellowship from the National Foundation for Infantile Paralysis.

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Molecular Structure of Deoxyribose Nucleic Acids

WHILE the biological properties of deoxyribose nucleic acid suggest a molecular structure containing great complexity, X-ray diffraction studies described here (cf. Astbury¹) show the basic molecular configuration has great simplicity. The purpose of this communication is to describe, in a preliminary way, some of the experimental evidence for the polynucleotide chain configuration being helical, and existing in this form when in the natural state. A fuller account of the work will be published shortly.

The structure of deoxyribose nucleic acid is the same in all species (although the nitrogen base ratios alter considerably) in nucleoprotein, extracted or in cells, and in purified nucleate. The same linear group of polynucleotide chains may pack together parallel in different ways to give crystalline²⁻³, semi-crystalline or paracrystalline material. In all cases the X-ray diffraction photograph consists of two regions, one determined largely by the regular spacing of nucleotides along the chain, and the other by the longer spacings of the chain configuration. The sequence of different nitrogen bases along the chain is not made visible.

Oriented paracrystalline deoxyribose nucleic acid ('structure B' in the following communication by Franklin and Gosling) gives a fibre diagram as shown in Fig. 1 (cf. ref. 4). Astbury suggested that the strong 3.4-A. reflexion corresponded to the internucleotide repeat along the fibre axis. The ~ 34 A. layer lines, however, are not due to a repeat of a polynucleotide composition, but to the chain configuration repeat, which causes strong diffraction as the nucleotide chains have higher density than the interstitial water. The absence of reflexions on or near the meridian immediately suggests a helical structure with axis parallel to fibre length.

Diffraction by Helices

It may be shown⁵ (also Stokes, unpublished) that the intensity distribution in the diffraction pattern of a series of points equally spaced along a helix is given by the squares of Bessel functions. A uniform continuous helix gives a series of layer lines of spacing corresponding to the helix pitch, the intensity distribution along the n th layer line being proportional to the square of J_n , the n th order Bessel function. A straight line may be drawn approximately through

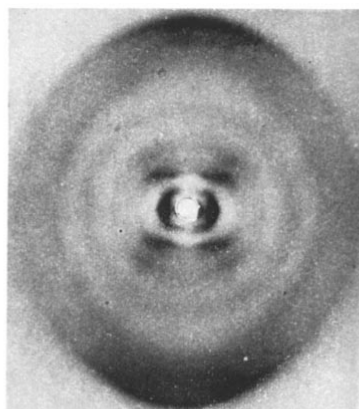


Fig. 1. Fibre diagram of deoxyribose nucleic acid from *B. coli*. Fibre axis vertical.

the innermost maxima of each Bessel function and the origin. The angle this line makes with the equator is roughly equal to the angle between an element of the helix and the helix axis. If a unit repeats n times along the helix there will be a meridional reflexion (J_0^2) on the n th layer line. The helical configuration produces side-bands on this fundamental frequency, the effect⁶ being to reproduce the intensity distribution about the origin around the new origin, on the n th layer line, corresponding to C in Fig. 2.

We will now briefly analyse in physical terms some of the effects of the shape and size of the repeat unit or nucleotide on the diffraction pattern. First, if the nucleotide consists of a unit having circular symmetry about an axis parallel to the helix axis, the whole diffraction pattern is modified by the form factor of the nucleotide. Second, if the nucleotide consists of a series of points on a radius at right-angles to the helix axis, the phases of radiation scattered by the helices of different diameter passing through each point are the same. Summation of the corresponding Bessel functions gives reinforcement for the inner-

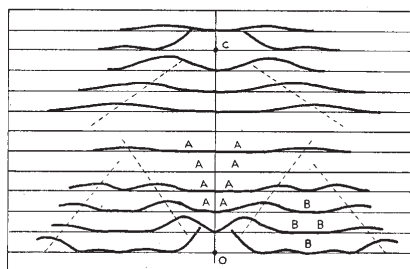


Fig. 2. Diffraction pattern of system of helices corresponding to structure of deoxyribose nucleic acid. The squares of Bessel functions are plotted about 0 on the equator and on the first, second, third and fifth layer lines for half of the nucleotide mass at 20 A. diameter and remainder distributed along a radius, the mass at a given radius being proportional to the radius. About C on the tenth layer line similar functions are plotted for an outer diameter of 12 A.