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The Scattering of Light by Uniformly Curved Rods. A Model of Semirigid Rod Macromolecules

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ABSTRACT: Uniformly curved rods may be used as a model of rodlike macromolecules which are not rigid enough to be straight rods in solution. The dependence of scattered light intensity upon scattering angle (form factor) has been obtained numerically for curved rods with angles of bend from 0 (straight rod) to 150°. The results have been used to synthesize "experimental" scattering data for rods with lengths from 1500 to 5000 Å, over the range of scattering angles accessible to conventional light-scattering photometers. The errors incurred in extrapolation of the inverse form factors to zero scattering angle are shown to be not excessive. Further, it is shown that in some circumstances the ratio of the scattered intensities at two supplementary angles is a function primarily of the contour length of the rod and does not depend strongly upon the angle of bend. Measuring such a ratio therefore gives an estimate of contour length and, if the relation between contour length and molecular weight is known, of molecular weight.

(I) Introduction

Light scattering has long been used to obtain information about molecular weights and size and shape parameters for DNA and other macromolecules.[1] Ultrasonically sheared DNA fragments, with molecular weights of the order of 10^5–10^6, have also been studied by light scattering and other techniques.[2,3] Molecular weight and mean-square radius may be obtained in principle by appropriate extrapolation of light-scattering data to the limit of zero scattering angle. In practice, the range of scattering angle accessible to conventional light-scattering photometers may not extend to sufficiently small scattering angles to permit reliable estimates of molecular weight and mean-square radius.[4,5] Interpretation of the angular dependence of the scattering is further complicated by lack of knowledge of the shapes of DNA chains. Thus, although the wormlike chain[6] is widely used as a model of DNA chains, agreement is lacking on the value of the model's

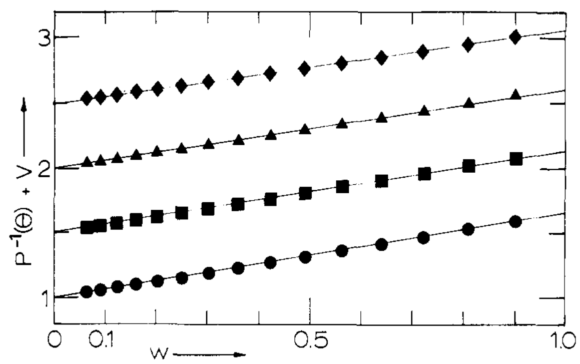

Figure 1. Inverse form factors $P^{-1}(\theta)$ vs. $w = \sin^2 \theta/2$, for light of wavelength in solution 4090 Å, scattered from uniformly curved rods of contour length 1500 Å, plotted with vertical offsets V for angles of bend ϕ as follows: (●) $\phi = 0°$ (straight rod), $V = 0$; (■) $\phi = 45°$, $V = 0.5$; (▲) $\phi = 90°$, $V = 1.0$; (♦) $\phi = 135°$, $V = 1.5$. The straight lines are visual estimates of the limiting linear behavior at small scattering angles, which are used to estimate molecular weight and mean-square radius.

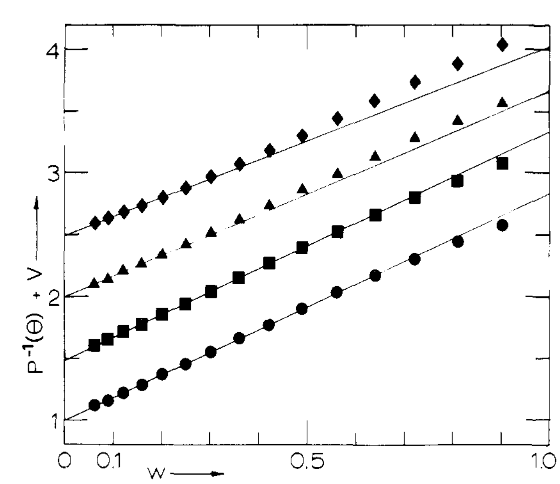

Figure 2. Inverse form factors for uniformly curved rods of contour length 2500 Å. The assumed wavelength of light, the vertical offsets, and the notation are the same as those in Figure 1.

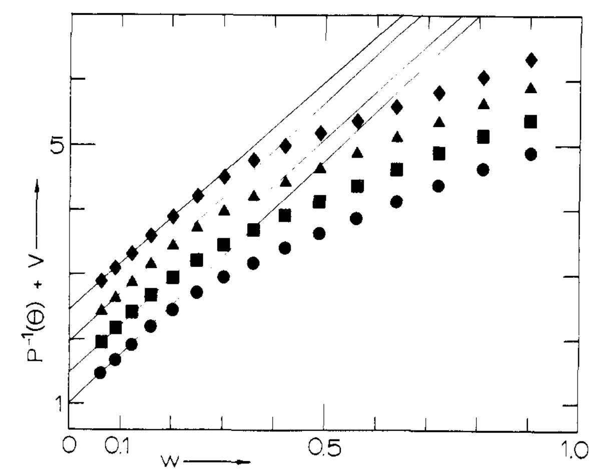

Figure 3. Inverse form factors for uniformly curved rods of contour length 5000 Å. The assumed wavelength of light, the vertical offsets, and the notation are the same as those in Figure 1.

characteristic stiffness parameter (persistence length) for DNA,[4,5,7] and the model itself may not be suitable for the shorter DNA fragments, whose persistence length in the wormlike chain model would be of the same order of magnitude as the contour length of the chain. In addition, calculations of the angular dependence of the scattering from the wormlike chain have either required the use of approximate distributions in intrachain separation[8,9] or been limited to persistence lengths less than or equal to the chain contour length.[10]

In this paper, we report the results of calculations of the angular dependence of the scattering of light from uniformly curved rods, i.e., circular arcs. While a uniformly curved rod is at best an imprecise model of the instantaneous shape of a semirigid rod such as a short DNA fragment in solution, it may well be as good a model as the wormlike chain for this purpose, and its scattering behavior can be calculated exactly for angles of bend as close to zero (the straight-rod limit) as desired. We first demonstrate the close agreement between the results obtained for the curved rod and for the wormlike chain when the contour length equals the persistence length. In order to estimate the extrapolation error inherent in the analysis of light-scattering data obtained for curved rods, we exhibit synthesized "experimental" data for arcs of various curvatures and contour lengths and estimate the extrapolation errors to which they give rise. We then report an apparent simplicity in the scattering at large angles which suggests the possibility of estimating the contour length of curved rods directly from the angular dependence of the scattering. Finally, we discuss the estimation of a persistence-length parameter for a curved rod from its contour length and mean-square radius.

(II) Method

For sufficiently dilute solutions, the angular dependence of the scattering from solute molecules may be expressed[11] in the form:

$$Kc/R_\theta = [MP(\theta)]^{-1} \quad (1)$$

where the Rayleigh ratio R_θ is an experimentally accessible quantity proportional to the intensity of light scattered through an angle θ, K contains the angular dependence due to system geometry and polarization but not that due to the size and shape of the scattering species, M is the (weight-average) molecular weight of the solute, c is the concentration (weight solute per unit volume solution), and the form factor $P(\theta)$ is normalized to approach unity in the limit of zero scattering angle. In this dilute-solution limit, $P(\theta)$ is given by

$$P(\theta) = \langle (\sin v_{ij})/v_{ij} \rangle \quad (2)$$

where $v_{ij} = 4\pi r_{ij} \sin(\theta/2)/\lambda$, λ is the wavelength of the incident radiation in the solution, r_{ij} is the distance between scattering centers i and j in the solute molecule, and the angular brackets denote the average over all pairs i and j and all possible orientations of the solute molecule.

At sufficiently small scattering angles, the reciprocal of $P(\theta)$ may be expanded in a Taylor series in v_{ij}:

$$\begin{aligned} P^{-1}(\theta) &= 1 + \tfrac{1}{6}\langle v_{ij}^2 \rangle + \ldots \\ &= 1 + \tfrac{1}{6}(4\pi/\lambda)^2 \langle r_{ij}^2 \rangle \sin^2 \theta/2 + \ldots \quad (3) \\ &= 1 + \tfrac{1}{3}(4\pi/\lambda)\rho^2 \sin^2 \theta/2 + \ldots \end{aligned}$$

where the mean-square radius ρ^2 is just half $\langle r_{ij}^2 \rangle$. Thus as the scattering angle approaches zero, a plot of Kc/R_θ vs. $\sin^2 \theta/2$ approaches a limiting value of $1/M$ and a limiting slope proportional to the mean-square radius of the solute macromolecules.

Form factors $P(\theta)$ and their reciprocals were calculated as functions of θ for rods of various contour lengths and angles

Table I
Results of Visual Extrapolation of the Form-Factor Plots Shown in Figures 1–3[a]

L, Å	ϕ, deg	θ_{max}, deg	$P^{-1}(\theta)$ at θ_{max}	True ρ, Å	Apparent ρ, Å	Apparent $P^{-1}(0)$ from intercept	% error in apparent values of ρ	% error in apparent values of M
1500	0	144	1.6	433	463	0.99	7	1
	45	144	1.6	429	453	1.00	6	0
	90	144	1.5	416	437	1.00	5	0
	135	144	1.5	395	426	0.99	8	1
2500	0	106	2.2	722	772	0.99	7	1
	45	106	2.2	714	778	0.98	9	2
	90	60	1.4	693	734	0.99	6	1
	135	53	1.3	658	699	0.99	6	1
5000	0	41	1.9	1443	1550	0.99	7	1
	45	41	1.9	1249	1558	0.98	9	2
	90	47	2.1	1385	1575	0.95	14	5
	135	60	2.7	1317	1533	0.95	16	5

[a] For curved rods of contour length L and angle of bend ϕ, for scattering angles θ in the range $29° \leq \theta \leq \theta_{max}$, where θ_{max} is the largest scattering angle for which the plot appears linear. The wavelength λ of light in the solution is taken as 4090 Å. The apparent molecular weight M is inversely proportional to the zero-angle intercept I of the limiting straight line, and the root-mean-square radius ρ (radius of gyration) is related to I and the limiting slope S by $\rho = (3S/I)^{1/2}\lambda/(4\pi)$.

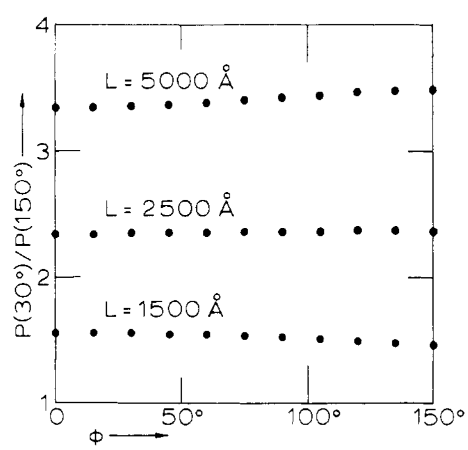

Figure 4. Ratios $P(30°)/P(150°)$ from Table III, plotted as a function of angle ϕ of bend, for contour lengths L of 1500, 2500, and 5000 Å.

of bend. At each value of θ, $P(\theta)$ was calculated from eq 2, the average being obtained by numerical integration. The computational details are given in the Appendix. The results obtained are given in the following sections.

(III) Comparison with the Wormlike Chain

Yamakawa and Fujii[10] (hereafter referred to as YF) have calculated form factors for wormlike chains with contour lengths greater than or equal to the persistence length. In order to compare our results for the curved rod with theirs for the wormlike chain, we must first define a persistence length for the curved rod. The definition will of necessity be an arbitrary one, but since we wish to compare light-scattering form factors, it seems natural to define the persistence length of a curved rod through its mean-square radius. A curved rod is characterized by its contour length L and the angle ϕ between its initial and final direction; its ratio ρ^2/L^2 of mean-square radius to the square of contour length is a function of ϕ. In the YF treatment, the shape of a chain is characterized by the ratio x of its contour length to its persistence length. For a curved rod with a given value of ρ^2/L^2, we define x as the value for which the YF treatment gives the same value of ρ^2/L^2.

For a wormlike chain, ρ^2/L^2 is given[12] by

$$\rho^2/L^2 = 2x^{-4}\,[\exp(-x) - (1 - x + x^2/2! - x^3/3!)] \quad (4)$$

Table II
Results of Extrapolations Similar to Those of Table I, but with θ_{max} Taken as the Largest Scattering Angle for Which $P^{-1}(\theta) \leq 1.3$

L, Å	ϕ, deg	θ_{max}, deg	True ρ, Å	Apparent ρ, Å	% error in apparent ρ
1500	0	81	433	449	4
	45	81	429	444	3
	90	89	416	434	4
	135	89	395	414	5
2500	0	47	722	756	5
	45	47	714	749	5
	90	47	693	749	5
	135	47	658	694	5

The smallest value of x (least-flexible chain) for which form factors are tabulated by YF is $x = 1$, for which eq 4 gives $\rho^2/L^2 = 0.06909$. For a curved rod, we can easily derive the relation

$$\rho^2/L^2 = \phi^{-2}[1 - (\phi/2)^{-2}\sin^2\phi/2] \quad (5)$$

which gives $\phi = 136.38°$ for $\rho^2/L^2 = 0.06909$. The largest scattering angle θ for which YF have tabulated form factors is given by $\theta = 2\sin^{-1}[11^{1/2} \times \lambda/(8\pi L)]$, where λ is the wavelength of light in the solution. For example, for $\lambda = 4090$ Å, the wavelength of the green mercury line in water, and for a chain with contour length and persistence length both equal to 1410 Å, this maximum value of θ is 45°, a readily accessible value experimentally. For this scattering angle, the wormlike chain form factor given by YF is 0.9393. For a curved rod with the corresponding angle of bend and scattering angle, the form factor was found from eq 2 to be 0.9392. This extremely close agreement is due in large part to the fact that we are comparing chains with the same mean-square radius, thus forcing agreement of the first two terms in the Taylor-series expansions for the form factor in the two models. In order to examine the difference between the model-dependent parts of the form factors, we should therefore subtract $1 - \frac{1}{3}[(4\pi/\lambda)\sin\theta/2]^2\rho^2$. For the data we have assumed, this expression has the value 0.9367. Thus the model-dependent part of the form factor is 0.0026 for the YF treatment and 0.0025 for the curved rod. This difference of about 4% may be taken as a measure of the agreement between the two models for a chain with a contour length equal to its persistence length.

Table III
Ratios $P(30°)/P(150°)$ of Light Scattered at 30 and 150° by Uniformly Curved Rods of Contour Lengths L and Angles of Bend ϕ Shown, Taking the Wavelength of Light in the Solution to be 4090 Å

	ϕ, deg										
L, Å	0	15	30	45	60	75	90	105	120	135	150
600	1.08	1.08	1.08	1.08	1.08	1.08	1.08	1.07	1.07	1.07	1.07
1000	1.24	1.24	1.24	1.23	1.23	1.23	1.22	1.21	1.21	1.20	1.19
1500	1.55	1.55	1.55	1.54	1.54	1.53	1.52	1.51	1.49	1.48	1.46
2000	1.95	1.95	1.95	1.95	1.94	1.94	1.93	1.92	1.91	1.89	1.87
2300	2.20	2.20	2.20	2.20	2.20	2.20	2.19	2.19	2.18	2.17	2.16
2500	2.34	2.34	2.35	2.35	2.35	2.36	2.36	2.36	2.37	2 37	2.36
2700	2.47	2.47	2.48	2.48	2.49	2.50	2.51	2.52	2.53	2.54	2.55
3000	2.64	2.64	2.64	2.65	2.66	2.67	2.69	2.71	2.74	2.77	2.80
3500	2.86	2.86	2.86	2.87	2.88	2.89	2.91	2.93	2.97	3.01	3.06
4000	3.06	3.06	3.06	3.07	3.07	3.08	3.09	3.11	3.13	3.15	3.20
4500	3.23	3.23	3.24	3.24	3.25	3.26	3.27	3.28	3.29	3.30	3.32
5000	3.34	3.34	3.35	3.36	3.38	3.40	3.42	3.44	3.46	3.47	3.48
6000	3.44	3.44	3.45	3.46	3.47	3.49	3.52	3.56	3.61	3.68	3.75
7000	3.48	3.48	3.48	3.49	3.51	3.52	3.54	3.56	3.58	3.62	3.69
8000	3.46	3.46	3.46	3.47	3.48	3.49	3.51	3.54	3.57	3.60	3.61
9000	3.46	3.46	3.46	3.46	3.46	3.46	3.46	3.47	3.48	3.52	3.57
10000	3.47	3.47	3.47	3.47	3.46	3.46	3.46	3.45	3.44	3.43	3.43
15000	3.60	3.60	3.60	3.60	3.60	3.61	3.62	3.63	3.62	3.62	3.62

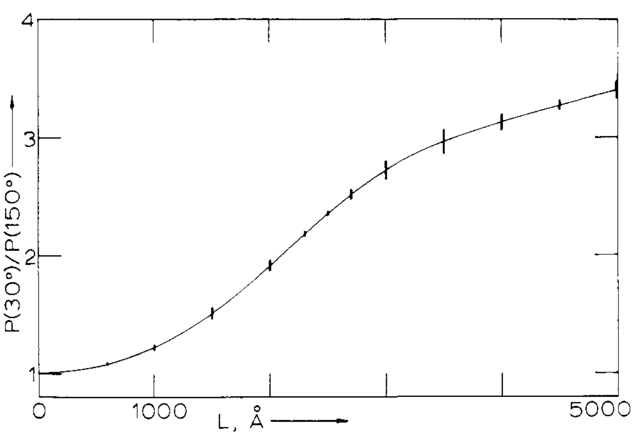

Figure 5. Ratios $P(30°)/P(150°)$ from Table III, plotted as a function of contour length L. At each value of L, the vertical bar shows the range of values of the ratio as the angle ϕ of bend is varied from 0 (straight rod) to 150°.

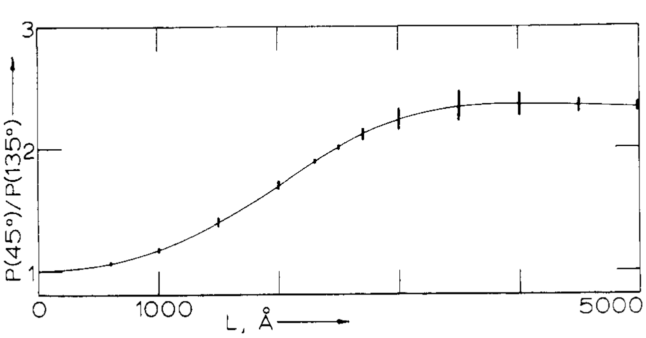

Figure 6. Ratios $P(45°)/P(135°)$ from Table IV, plotted as a function of contour length L. At each value of L, the vertical bar shows the range of values of the ratio as the angle ϕ of bend is varied from 0° (straight rod) to 150°.

Table IV
Uncertainty ΔL in Values of Contour Length L of Curved Rods Estimated from the Dissymmetry Ratios $P(30°)/P(150°)$ and $P(45°)/P(135°)$, and the Relative Uncertainties $\Delta L/L$ (%), Assuming the Wavelength of Light in the Solution is 4090 Å

	Estimator			
	$P(30°)/P(150°)$		$P(45°)/P(135°)$	
L, Å	ΔL, Å	$\Delta L/L$, %	ΔL, Å	$\Delta L/L$, %
600	39	6	95	16
1000	120	12	100	10
1500	120	8	130	9
2000	100	5	90	5
2300	40	2	33	1
2500	40	2	53	2
2700	100	4	180	7
3000	260	9		
3500	500	14		
4000	440	11		
4500	330	7		
5000	540	11		

(IV) Form Factor Extrapolation Errors

Figures 1–3 show reciprocal form factors $P^{-1}(\theta)$, calculated from eq 2 as previously described, for curved rods with contour lengths L of 1500, 2500, and 5000 Å, with the wavelength of light in the solution taken as 4090 Å, and bending angles ϕ of 45, 90, and 135°. The results for straight rods (ϕ = 0°), which can of course be calculated directly, without the necessity of numerical integration, are also shown. Values of $P^{-1}(\theta)$ are given for 15 scattering angles θ from 29 to 144°, corresponding roughly to the angular range accessible to light-scattering photometers not specially designed to study small-angle scattering.

For each of the form factors in Figures 1–3, the limiting straight-line behavior at small angles was estimated visually. For plots of experimental values of Kc/R_θ vs. $\sin^2 \theta/2$, an estimate of molecular weight would be obtained from the zero-angle intercept of the limiting straight line, and an estimate of the mean-square radius would be obtained from the ratio of its slope to its intercept. Table I shows the values of root-mean-square radius (radius of gyration) ρ obtained from the straight-line estimates shown in Figures 1–3, together with the true values of ρ and the errors in M and ρ resulting from the straight-line estimates.

Table I also shows the maximum scattering angles θ_{max} for which $P^{-1}(\theta)$ appeared to be a linear function of $\sin^2 \theta/2$, and the corresponding values of $P^{-1}(\theta_{max})$, which range from 1.3 to 2.7. The condition $P^{-1}(\theta_{max}) \leq 1.3$ has been used[5] as a cri-

Table V
Dissymmetry Ratios $P(45°)/P(135°)$ of Light Scattered at 45 and 135° by Uniformly Curved Rods of Contour Lengths L and Angles of Bend ϕ Shown, Taking the Wavelength of Light in the Solution to be 4090 Å

	ϕ, deg										
L, Å	0	15	30	45	60	75	90	105	120	135	150
600	1.07	1.07	1.07	1.07	1.07	1.06	1.06	1.06	1.06	1.06	1.05
1000	1.19	1.19	1.19	1.19	1.18	1.18	1.18	1.17	1.17	1.16	1.15
1500	1.43	1.43	1.43	1.42	1.42	1.41	1.41	1.40	1.39	1.38	1.36
2000	1.73	1.73	1.73	1.72	1.72	1.72	1.71	1.70	1.69	1.68	1.67
2300	1.90	1.90	1.90	1.90	1.90	1.90	1.90	1.90	1.90	1.89	1.88
2500	1.99	1.99	1.99	2.00	2.00	2.01	2.01	2.02	2.02	2.02	2.02
2700	2.07	2.07	2.07	2.08	2.09	2.10	2.11	2.12	2.14	2.15	2.16
3000	2.15	2.15	2.16	2.17	2.18	2.19	2.21	2.23	2.26	2.29	2.32
3500	2.22	2.22	2.23	2.24	2.25	2.27	2.29	2.32	2.35	2.40	2.46
4000	2.26	2.26	2.27	2.27	2.28	2.29	2.31	2.33	2.36	2.40	2.45
4500	2.29	2.29	2.29	2.29	2.30	2.31	2.32	2.33	2.35	2.37	2.40
5000	2.29	2.29	2.29	2.30	2.31	2.32	2.33	2.34	2.35	2.36	2.37
6000	2.26	2.26	2.26	2.26	2.27	2.27	2.28	2.29	2.31	2.33	2.36
7000	2.28	2.28	2.28	2.28	2.27	2.27	2.26	2.25	2.24	2.24	2.25
8000	2.31	2.31	2.31	2.31	2.31	2.30	2.30	2.29	2.27	2.24	2.20
9000	2.34	2.34	2.34	2.34	2.34	2.33	2.33	2.32	2.32	2.31	2.28
10000	2.34	2.35	2.35	2.35	2.35	2.36	2.36	2.36	2.35	2.35	2.35
15000	2.37	2.37	2.37	2.37	2.37	2.37	2.37	2.36	2.35	2.34	2.34

terion of the region in which to expect limiting linear behavior. The extrapolations were therefore repeated for rods of contour length 1500 and 2500 Å, letting θ_{max} be the largest scattering angle for which $P^{-1}(\theta_{max}) \leq 1.3$. (For a contour length of 5000 Å, $P^{-1}(29°)$ is already greater than 1.3.) The values of ρ obtained from these extrapolations are given in Table II, together with their errors.

(V) Dissymmetry Ratios

The form factors obtained from the calculations of the preceding section at large scattering angles appear to depend primarily upon the contour length of the rod and to be relatively insensitive to its angle of bend. We therefore investigated the possibility of using the ratio of the scattering at a large angle to the scattering at its supplementary angle (a generalized dissymmetry ratio) as a measure of contour length. Ratios $P(30°)/P(150°)$ were calculated for rods of lengths from 600 to 15 000 Å and for angles of bend from 0 (straight rod) to 150°. The results are given in Table III. Figure 4 shows the data of Table III for three lengths, plotted as $P(30°)/P(150°)$ vs. ϕ. The relatively small variation of the ratio with ϕ for a given contour length is evident. It also appears from Table III that the ratio increases with increasing contour length up to about 5000 Å and then remains more or less constant. Figure 5 shows the data of Table III for contour lengths up to 5000 Å, replotted to show the dependence of $P(30°)/P(150°)$ upon contour length. For each contour length, the vertical bar in Figure 5 shows the range of values of $P(30°)/P(150°)$ as ϕ varies from 0 to 150°. It is clear that for contour lengths between 1000 and 5000 Å, the ratio $P(30°)/P(150°)$ can be used to obtain at least an approximate estimate of contour length. For macromolecules such as DNA, for which estimates of the ratio of contour length to molecular weight are available, molecular weight may therefore be estimated from the ratio of the scattering at two angles, without the need for extrapolation to zero scattering angle or for determining the absolute scattering. Table IV shows the uncertainties in contour lengths estimated in this way, based on the range of the vertical bars in Figure 5 and the local slope of the smooth curve drawn (by eye) through them.

The more usual dissymmetry ratio $P(45°)/P(135°)$, frequently employed to estimate molecular size,[13] was also obtained for bent rods. The results are given in Table V and are plotted as a function of contour length in Figure 6. It will be seen that this ratio may also be used to estimate contour lengths of bent rods up to about 3000 Å but that it ceases to be sensitive to contour length beyond this point. The uncertainties in contour lengths estimated in this way are given in Table IV.

(VI) Estimation of Persistence Length

In sections IV and V we showed that under some circumstances it is possible to estimate the mean-square radius and the contour length of curved rods from the limiting small-angle scattering and ratios of large- to small-angle scattering, respectively. We now consider the possibility of using mean-square radius and contour length together to estimate persistence length. In principle, if we adopt the definition of a persistence length for a curved rod employed in section III, we can obtain the persistence length of a chain for which ρ and L are known by solving eq 4 for x. However, the right-hand side of eq 4 is a rather slowly varying function of x in the region $0 \leq x \leq 2$. For x in the region of 1, a 5% error in ρ^2/L^2 gives rise to a 30% error in x. In view of the expected errors in ρ and L given in Tables II and IV, it appears that a very rough estimate of persistence length is the best one can hope for.

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Appendix

For a uniformly curved rod of contour length L and total angle of bend ϕ, the expression in eq 2 for the form factor $P(\theta)$ may be written in the form:

$$P(\theta) = 2\int_0^1 (1 - \xi) j_0[4\pi v \xi j_0(\xi\phi/2)]\, d\xi \qquad (A1)$$

$j_0(z) = \sin z/z$, $\xi = r/L$, r is contour length along the rod, $v = (L/\lambda) \sin \theta/2$, λ is the wavelength of light in the solution, and θ is the scattering angle.

Table VI

Light-Scattering Form Factors $P(\theta)$ for Curved Rods with Total Angle of Bend ϕ, as a Function of the Variable $v = (L/\lambda) \sin \theta/2$, where L is Contour Length, λ is the Wavelength of Light in the Solution, and θ is the Scattering Angle

v \ ϕ	0°	15°	30°	45°	60°	75°	90°	105°	120°	135°	150°
.01	.9996	.9996	.9996	.9996	.9996	.9996	.9996	.9996	.9996	.9996	.9996
.02	.9982	.9982	.9983	.9983	.9983	.9983	.9984	.9984	.9985	.9985	.9986
.03	.9961	.9961	.9961	.9961	.9962	.9963	.9964	.9965	.9966	.9967	.9969
.04	.9930	.9930	.9931	.9932	.9933	.9934	.9936	.9937	.9940	.9942	.9944
.05	.9891	.9891	.9892	.9893	.9895	.9897	.9900	.9903	.9906	.9909	.9913
.06	.9844	.9844	.9845	.9847	.9849	.9852	.9856	.9860	.9865	.9870	.9875
.07	.9788	.9789	.9790	.9793	.9796	.9800	.9805	.9810	.9816	.9823	.9830
.08	.9725	.9725	.9727	.9730	.9734	.9740	.9746	.9753	.9761	.9770	.9779
.09	.9654	.9654	.9657	.9660	.9666	.9672	.9680	.9689	.9699	.9710	.9722
.10	.9575	.9576	.9579	.9583	.9589	.9597	.9607	.9618	.9630	.9643	.9658
.12	.9396	.9397	.9401	.9408	.9416	.9427	.9441	.9456	.9473	.9492	.9512
.14	.9191	.9193	.9198	.9206	.9218	.9232	.9249	.9269	.9292	.9315	.9343
.16	.8963	.8965	.8971	.8982	.8996	.9014	.9035	.9060	.9088	.9119	.9153
.18	.8715	.8718	.8725	.8737	.8754	.8775	.8801	.8831	.8865	.8902	.8943
.20	.8450	.8453	.8461	.8475	.8495	.8520	.8550	.8585	.8624	.8668	.8716
.22	.8172	.8175	.8184	.8200	.8222	.8250	.8284	.8324	.8369	.8419	.8474
.24	.7884	.7887	.7897	.7915	.7939	.7970	.8007	.8051	.8102	.8158	.8219
.26	.7589	.7593	.7604	.7622	.7648	.7682	.7722	.7770	.7825	.7886	.7954
.28	.7291	.7295	.7307	.7326	.7354	.7389	.7432	.7482	.7541	.7607	.7680
.30	.6994	.6998	.7010	.7030	.7058	.7094	.7139	.7192	.7253	.7323	.7401
.32	.6699	.6703	.6715	.6735	.6764	.6801	.6846	.6901	.6964	.7036	.7118
.34	.6410	.6414	.6426	.6446	.6474	.6511	.6557	.6611	.6676	.6750	.6833
.36	.6130	.6133	.6145	.6164	.6192	.6228	.6273	.6327	.6391	.6465	.6550
.38	.5859	.5862	.5873	.5892	.5918	.5952	.5996	.6049	.6112	.6185	.6270
.40	.5600	.5603	.5613	.5630	.5655	.5687	.5729	.5779	.5840	.5912	.5995
.42	.5354	.5357	.5366	.5382	.5404	.5434	.5472	.5519	.5577	.5646	.5727
.44	.5122	.5125	.5133	.5147	.5166	.5193	.5228	.5271	.5325	.5390	.5467
.46	.4905	.4907	.4914	.4926	.4943	.4966	.4997	.5036	.5085	.5144	.5216
.48	.4702	.4704	.4710	.4719	.4734	.4754	.4780	.4814	.4857	.4911	.4977
.50	.4514	.4516	.4520	.4528	.4539	.4555	.4577	.4606	.4643	.4690	.4749
.52	.4341	.4342	.4345	.4351	.4359	.4372	.4389	.4412	.4442	.4482	.4534
.54	.4181	.4182	.4184	.4188	.4194	.4202	.4215	.4232	.4256	.4289	.4333
.56	.4035	.4035	.4036	.4038	.4041	.4047	.4054	.4066	.4084	.4109	.4144
.58	.3900	.3900	.3901	.3901	.3902	.3904	.3908	.3914	.3925	.3943	.3970
.60	.3777	.3777	.3777	.3776	.3774	.3774	.3773	.3775	.3780	.3790	.3809
.62	.3664	.3664	.3663	.3661	.3658	.3655	.3651	.3648	.3648	.3651	.3661
.64	.3561	.3560	.3558	.3555	.3551	.3546	.3540	.3533	.3527	.3524	.3526
.66	.3464	.3464	.3462	.3458	.3453	.3446	.3438	.3428	.3418	.3409	.3403
.68	.3375	.3375	.3372	.3369	.3363	.3355	.3345	.3333	.3319	.3305	.3293
.70	.3292	.3291	.3289	.3285	.3279	.3271	.3260	.3246	.3230	.3212	.3193
.72	.3214	.3213	.3211	.3207	.3201	.3193	.3182	.3167	.3149	.3127	.3104
.74	.3139	.3139	.3137	.3134	.3128	.3120	.3109	.3094	.3075	.3051	.3023
.76	.3069	.3068	.3067	.3064	.3059	.3052	.3041	.3027	.3007	.2981	.2951
.78	.3001	.3000	.2999	.2997	.2993	.2987	.2978	.2964	.2944	.2919	.2886
.80	.2935	.2935	.2934	.2933	.2930	.2925	.2917	.2904	.2886	.2861	.2828
.82	.2872	.2872	.2871	.2871	.2869	.2865	.2859	.2848	.2832	.2808	.2775
.84	.2810	.2810	.2810	.2810	.2809	.2807	.2803	.2794	.2780	.2758	.2727
.86	.2750	.2750	.2751	.2751	.2751	.2751	.2748	.2742	.2731	.2711	.2682
.88	.2692	.2692	.2693	.2694	.2695	.2696	.2695	.2691	.2683	.2667	.2640
.90	.2635	.2635	.2636	.2638	.2640	.2642	.2643	.2641	.2636	.2623	.2600
.92	.2579	.2580	.2581	.2583	.2585	.2588	.2591	.2592	.2590	.2581	.2562
.94	.2526	.2526	.2527	.2530	.2533	.2536	.2540	.2544	.2544	.2539	.2525
.96	.2474	.2474	.2475	.2478	.2481	.2485	.2490	.2495	.2499	.2498	.2488
.98	.2423	.2424	.2425	.2427	.2431	.2435	.2441	.2448	.2454	.2456	.2451
1.00	.2375	.2375	.2376	.2378	.2382	.2387	.2393	.2401	.2409	.2415	.2414
1.05	.2262	.2262	.2263	.2264	.2267	.2271	.2277	.2286	.2297	.2310	.2320
1.10	.2161	.2161	.2161	.2162	.2163	.2165	.2169	.2177	.2189	.2204	.2222
1.15	.2072	.2072	.2071	.2071	.2070	.2070	.2072	.2077	.2086	.2101	.2122
1.20	.1991	.1991	.1990	.1989	.1988	.1986	.1985	.1986	.1991	.2003	.2023
1.25	.1918	.1918	.1917	.1916	.1914	.1911	.1908	.1906	.1906	.1912	.1928
1.30	.1850	.1850	.1850	.1849	.1847	.1844	.1841	.1836	.1832	.1832	.1840
1.35	.1786	.1786	.1786	.1786	.1785	.1783	.1779	.1774	.1767	.1761	.1762
1.40	.1725	.1725	.1725	.1725	.1725	.1725	.1723	.1718	.1710	.1701	.1694
1.45	.1666	.1666	.1667	.1668	.1668	.1669	.1669	.1666	.1660	.1649	.1637
1.50	.1611	.1611	.1611	.1612	.1614	.1615	.1617	.1616	.1613	.1603	.1589
1.55	.1559	.1559	.1559	.1560	.1561	.1563	.1566	.1568	.1567	.1561	.1547
1.60	.1511	.1511	.1511	.1511	.1512	.1514	.1517	.1520	.1522	.1521	.1510
1.65	.1466	.1466	.1466	.1466	.1466	.1467	.1469	.1473	.1478	.1480	.1475
1.70	.1425	.1425	.1425	.1424	.1424	.1424	.1425	.1428	.1434	.1439	.1440
1.75	.1387	.1387	.1387	.1386	.1385	.1384	.1384	.1386	.1390	.1398	.1404
1.80	.1351	.1351	.1350	.1350	.1349	.1347	.1346	.1346	.1349	.1356	.1366
1.85	.1316	.1316	.1316	.1315	.1315	.1313	.1311	.1310	.1311	.1316	.1327
1.90	.1282	.1282	.1282	.1282	.1282	.1281	.1279	.1277	.1275	.1278	.1288
1.95	.1250	.1250	.1250	.1250	.1251	.1250	.1249	.1246	.1243	.1243	.1250
2.00	.1218	.1219	.1219	.1219	.1220	.1220	.1220	.1218	.1214	.1211	.1214
2.10	.1161	.1161	.1161	.1161	.1162	.1163	.1164	.1164	.1162	.1156	.1151
2.20	.1110	.1110	.1109	.1109	.1109	.1109	.1111	.1113	.1114	.1111	.1102
2.30	.1063	.1063	.1063	.1063	.1062	.1062	.1062	.1063	.1066	.1068	.1063
2.40	.1020	.1020	.1020	.1020	.1020	.1019	.1018	.1018	.1020	.1024	.1026
2.50	.0980	.0980	.0980	.0980	.0981	.0981	.0980	.0978	.0977	.0980	.0987
2.60	.0942	.0942	.0942	.0943	.0943	.0944	.0944	.0943	.0941	.0940	.0945
2.70	.0908	.0908	.0908	.0908	.0908	.0908	.0909	.0910	.0909	.0905	.0906
2.80	.0877	.0877	.0877	.0877	.0876	.0876	.0876	.0878	.0878	.0876	.0871
2.90	.0847	.0847	.0847	.0847	.0847	.0847	.0846	.0847	.0849	.0849	.0844
3.00	.0819	.0819	.0819	.0820	.0820	.0820	.0819	.0818	.0819	.0822	.0820
3.10	.0793	.0793	.0793	.0793	.0794	.0794	.0794	.0793	.0792	.0795	.0797
3.20	.0769	.0769	.0769	.0769	.0769	.0769	.0770	.0769	.0768	.0768	.0772
3.30	.0746	.0746	.0746	.0746	.0746	.0746	.0746	.0747	.0746	.0744	.0747
3.40	.0725	.0725	.0725	.0725	.0724	.0724	.0724	.0725	.0725	.0723	.0722
3.50	.0704	.0704	.0704	.0704	.0704	.0704	.0703	.0704	.0705	.0704	.0701
3.60	.0684	.0684	.0685	.0685	.0685	.0685	.0685	.0684	.0685	.0686	.0683
3.70	.0666	.0666	.0666	.0666	.0666	.0667	.0667	.0666	.0666	.0668	.0667
3.80	.0649	.0649	.0649	.0649	.0649	.0649	.0649	.0649	.0648	.0649	.0651
3.90	.0633	.0633	.0633	.0633	.0633	.0632	.0633	.0633	.0633	.0632	.0635
4.00	.0617	.0617	.0617	.0617	.0617	.0617	.0617	.0617	.0618	.0616	.0617

The form factors given in this paper were evaluated by numerical integration of eq A1 on a digital computer, using single-precision floating point (27-bit fraction) arithmetic. The integrals were approximated with Simpson's rule, using 1000 intervals.

Four checks were made of the calculated form factors, as follows:

1. The calculated values of $P(0)$ were compared with unity. The maximum difference found was 4×10^{-6}.

2. For a straight rod, the right-hand side of eq A1 reduces to $Si(4\pi v)/(2\pi v) - j_0^2(2\pi v)$, where $Si(z)$ is the sine-integral function. Calculated values of $P(\theta)$ for $\phi = 0$ were compared with values hand calculated from tabulated[14] values of $Si(z)$ and $j_0(z)$, for selected values of v from 0.1 to 0.8. The maximum difference found was 4×10^{-6}.

3. Selected calculations of $P(\theta)$ were repeated using 500 intervals and 2000 intervals in the numerical integrations. The maximum changes in $P(\theta)$ were 4×10^{-6}.

4. Selected calculations of $P(\theta)$ were repeated using double-precision arithmetic. The maximum changes in $P(\theta)$ were 4×10^{-7}.

It is clear from the form of eq A1 that for a given value of θ the form factor is a function only of the variable v. As a matter of convenience, the calculations reported on the body of this paper were carried out for the values of v corresponding to the cited values of L, λ, and θ. Results at other values may readily be obtained from Table VI, in which $P(\theta)$ is given as a function of v and θ for values of v from zero to 4 and angles of bend from zero to 150°.

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