MODELLING BIOLOGICAL MACROMOLECULES IN SOLUTION: THE GENERAL TRI-AXIAL ELLIPSOID CAN NOW BE EMPLOYED

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Biological macromolecules, on the evidence of X-ray crytallography, have a complex three-dimensional shape which is thought to be little changed in solution. Our ability to describe the properties of such solutions is restricted though to certain simple models, to which we must approximate the real particles. The 'ellipsoid of revolution' (or bi-axial ellipsoid) has been widely used in biochemistry, the necessary mathematical solutions for the frictional and for the viscous flow properties having been obtained by Perrin (1) and by Simha (2) and Saito (3) respectively. The tri-axial ellipsoid would however be a much more realistic model. Recently (4) Perrin's equations have been solved numerically to cover this case: we have now derived a new equation for the viscous flow of dispersions of tri-axial ellipsoids. Much more realistic representation of the solution properties of biological fluids and of purified biopolymers thus becomes possible. Our solution takes the form:

$$\nu = \frac{1}{abc}\left\{\frac{4(\alpha_0'' + \beta_0'' + \gamma_0'')}{15(\beta_0''\gamma_0'' + \gamma_0''\alpha_0'' + \alpha_0''\beta_0'')} + \frac{1}{5}\left\{\frac{\beta_0 + \gamma_0}{\alpha_0'(b^2\beta_0 + c^2\gamma_0)} + \frac{\gamma_0 + \alpha_0}{\beta_0'(c^2\gamma_0 + a^2\alpha_0)} + \frac{\alpha_0 + \beta_0}{\gamma_0'(a^2\alpha_0 + b^2\beta_0)}\right\}\right\}$$

where ν is the conventionally defined viscosity increment, a, b and c are the three semi-axes, and the functions α_0 etc. are elliptic integrals defined by Jeffery (5). Values for ν over a limited range are given in the table. For the bi-axial cases the equation and hence the numerical values become identical to the Simha/Saito solution. A full derivation of this new equation together with details of the algorithms used for computation of the values for ν is to be submitted for publication elsewhere (6).

Table of values of a/b against b/c of the function ν for a general triaxial ellipsoid (a>b>c).

	a/b \ b/c	Prolate ellipsoid 1	2	3	4	5	6	7	8	9	10
Oblate ellipsoid	1	2.500	2.854	3.431	4.059	4.708	5.367	6.032	6.700	7.371	8.043
	2	2.908	3.803	4.857	5.951	7.060	8.176	9.298	10.422	11.548	12.675
	3	3.685	5.229	6.913	8.633	10.367	12.108	13.853	15.601	17.351	19.102
	4	4.663	6.986	9.440	11.926	14.427	16.934	19.446	21.960	24.476	26.993
	5	5.806	9.037	12.393	15.777	19.176	22.582	25.992	29.405	32.820	36.235
	6	7.099	11.363	15.744	20.155	24.579	29.010	33.445	37.883	42.322	46.762
	7	8.533	13.953	19.483	25.041	30.612	36.190	41.771	47.355	52.941	58.527
	8	10.103	16.798	23.595	30.420	37.256	44.098	50.944	57.793	64.643	71.494
	9	11.804	19.891	28.072	36.277	44.494	52.717	60.943	69.171	77.401	85.632
	10	13.634	23.227	32.904	42.604	52.314	62.030	71.749	81.470	91.193	100.916

The values quoted are immediately usable to test assumed models. Their use to infer the shape properties of biological macromolecules from measured hydrodynamic parameters might seem to be very questionable, as it has long been notorious that shape parameters even for the bi-axial case vary only slowly with shape, making the precision of retrieved 'axial ratios' poor. However a recently derived theory (7) has shown that a new shape parameter involving the transport-concentration dependence parameter varies rather rapidly with shape. We have therefore found it possible to devise procedures whereby the three principal semi-axes can be estimated without assumptions concerning the hydrodynamic volume (6).

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