# MODELLING BIOLOGICAL MACROMOLECULES IN SOLUTION: THE GENERAL TRI-AXIAL ELLIPSOID

**Stephen Ernest Harding, M.A. (Oxon), M.Sc.**

**PhD Dissertation**

**University of Leicester**

**1980**

Appendix VII Comparison of the radius of gyration for a sphere of uniform mass with that for a sphere of the same mass but with a spherical cavity

The radius of gyration, $R_G$ of a sphere of uniform mass and radius R is given by:

$$R_G^2 = \int_0^R 4\pi r^4 \, dr \Big/ \int_0^R 4\pi r^2 \, dr = \frac{3}{5}R^2 \qquad \text{(i)}$$

(Tanford, p 306, 1961). The radius of gyration of a spherical shell of uniform mass with radius $R_2$ and with a centrally placed spherical cavity of radius $R_1$ is given by:

$$R_G^2 = \int_{R_1}^{R_2} 4\pi r^4 \, dr \Big/ \int_{R_1}^{R_2} 4\pi r^2 \, dr = \frac{3}{5}\left(\frac{R_2^5 - R_1^5}{R_2^3 - R_1^3}\right) \qquad \text{(ii)}$$

The results of electron microscopy and x-ray diffraction (Harrison, 1959, Farrant, 1954, Kuff & Dalton, 1957, Labaw & Wycoff, 1957) suggest that apoferritin consists of twenty four sub-units, each of molecular weight 20,000, arranged in the form of a spherical shell of diameter 109 Å. If we take the radius of the hollow to be 18.5 Å, and the outer radius of the shell to be 54.5 Å, $R_G$ is calculated using formula (ii) to be 43.0 Å. The radius of gyration, had the same mass been concentrated into a uniform sphere of density identical to the shell would have been 41.6 Å, using formula (i); i.e. a discrepancy of $\sim 3.4\%$

# BIBLIOGRAPHY.

Alexander, A.E. and Johnson, P. (1949)

'Colloid Science', Volume 2, Oxford University Press

Alpert, S.S. and Banks, G. (1976)

Biophysical Chem. 4, 287

Baghurst, P.A., Nichol, L.W., Ogston, A.G., Winzor, D.J. (1975)

Biochem. J. 147, 575

Ballinger, K.W.A. and Jennings, B.R. (1979)

Nature 282, 699

Batchelor, G.K. (1967)

'An Introduction to Fluid Mechanics', Cambridge University Press

Batchelor, G.K. (1970)

J. Fluid Mech. 41, 545

Batchelor, G.K. and Green, J.T. (1972)

J. Fluid Mech. 56, 375

Beeman, W.W., Koesberg, P., Anderegg, J.W. and Webb, M.B. (1957)

in 'Handbuck der Physik', (Flugge, S. ed.), 32, 321, Springer-Verlagg (Berlin)

Benoit, H. (1951)

Ann. Physik. 6, 561

Berne, P.J. and Pecora, R. (1974)

Ann. Rev. Phys. Chem. 25, 233

Blake, C.C.F. (1975)

Essays in Biochem. II, 37

Blake, C.C.F., Geisow, M.J. and Oatley, S.J. (1978)

J. Mol. Biol. 121, 339

Blake, C.C.F., Koenig, D.F., Mair, G.A., North, A.C.T., Phillips, D.C. and Sarma, V.R. (1965)

Nature 206, 757

Bloomfield, V.A., Dalton, W.O. and Van Holde, K.E. (1967)

Biopolymers 5, 135

Bresler and Talmud (1944)

CR Acad. Sci. URSS, 43, 310

Brinkman, H.C., Hermans, J.J., Oosterhoff, L.J., Overbeek, J. Th. G., Polder, D., Staverman, A.J. and Wiebenga, E.H. (1949)

Proc. Int. Rheol. Congress (Schveningen) II, 77

Brenner, H. (1970)

J. Coll. Int. Sci. 32, 141

Brenner, H. (1972a)

Chem. Eng. Sci. 27, 1069

Brenner, H. (1972b)

Progr. Heat and Mass Transfer 5, 93

Cantor, C.R. and Tao, T. (1971)

Proc. Nucl. Acid Res. 2, 31

Cerf, R. and Scheraga, H.A. (1952)

Chem. Revs. 51, 185

Chapman, P.F. (1913)

Phil. Mag. 25, 475

Cheng, P.Y. and Schachman, H.K. (1955)

J. Polymer Sci. 16, 19

Chu, B. (1974)

'Laser Light Scattering', Academic, New York

Chwang, A.T. (1975)

J. Fluid Mech. 72, 17

Clenshaw, C.W. and Curtis, A.R. (1960)

Num. Math. 2, 197

Creeth, J.M. and Knight, C.G. (1965)
Biochim. Biophys. Acta 102, 549

Cummings, H.Z. and Pike, E.R. (1973)
(eds.) 'Photon Correlation and Light Beating Spectroscopy', Plenum, New York

Dickerson, R.E. and Geiss, I. (1969)
'The Structure and Action of Proteins', Benjamin, California

Dougherty, J. and Kreiger, I.M. (1972)
in Kreiger, Adv. Colloid Sci. 3, 111

Edsall, J.T. (1953)
in 'The Proteins' (Neurath, H. and Bailey, K. eds) 1B, Chapter 7, Academic, New York

Edwardes, D. (1892)
Quart. J. Math. 26, 70

Einstein, A. (1905)
Ann. Physik 17, 549

Einstein, A. (1906)
Ann. Physik 34, 591

Einstein, A. (1911)
Ann Physik 34, 591

Emes, C.H. (1977)

Ph. D. thesis, University of Leicester

Emes, C.H. and Rowe, A.J. (1978a)

Biochim. Biophys. Acta 537, 110

Emes, C.H. and Rowe, A.J. (1978b)

Biochim. Biophys. Acta 537, 125

Farrant, J.L. (1954)

Biochim. Biophys. Acta 13, 569

Feldman, R.J. (1976)

'Atlas of Macromolecular Structure on Microfiche', Traco Jitco Int., Rockville, Md. USA

Gans, R. (1928)

Ann. Physik 86, 628

Garcia Bernal, J.M. and Garcia de la Torre, J. (1980)

Biopolymers 19, 628

Garcia de la Torre, J. and Bloomfield, V.A. (1977a)

Biopolymers 16, 1747

Garcia de la Torre, J. and Bloomfield, V.A. (1977b)

Biopolymers 16, 1765

Garcia de la Torre, J. and Bloomfield, V.A. (1977c)

Biopolymers 16, 1779

Garcia de la Torre, J. and Bloomfield, V.A. (1978)

Biopolymers 17, 1605

Gardner, D.G., Gardner, J.C., Laush, G. and Meinke, W.W. (1959)

J. Chem. Phys. 31, 978

Giesekus, H. (1962)

Rheol. Acta 2, 50

Gill, P.E. and Murray, W. (1976)

Nat. Phys. Lab. report NAC 72

Gold, O. (1937)

Ph. D. thesis, University of Vienna

Goodwin, J.W. (1975)

Colloid Science 2 (Chemical Society), 246

Guoy, L.G. (1910)

J. Phys. Chem. 9, 457

Hall, C.E. and Slayter, H.S. (1959)

J. Biophys. Cytol. 5, 11

Harding, S.E. (1980a)

Biochem. J. 189 (in press)

Harding, S.E. (1980b)

mss. submitted to J. Phys. Chem.

Harrison, P.M. (1959)

J. Mol. Biol. 1, 69

Herzog, R.O., Illig, R. and Kudar, H. (1934)

Z. Phys. Chem. A167, 329

Holtzer, A. and Lowey, S. (1956)

J. Am. Chem. Soc. 78, 5954

Jablonski, A. (1961)

Naturforsch 169, 1

Jeffrey, G.B. (1922)

Proc. Roy. Soc. (London) A102, 476

Johnson, P. and Mihalyi, E. (1965)

Biochim. Biophys. Acta 102, 476

Jost, J.W. and O'Konski, C.T. (1978)

in 'Molecular Electro Optics' (O'Konski, C.T. ed.) Volume 2, 529

Kartha, G., Bello, J. and Harker, D. (1967)

Nature 213, 862

Kendrew, J.C., Bodo, G., Dintzis, H.M., Parrish, R.G., Wycoff, H. and Phillips, D.C. (1958)

Nature 181, 665

Kim, S.H. (1974)

in 'Biochemistry' (Stryer, L.) 653, Freeman, San Francisco

Kirkwood, J.G. (1967)

'Macromolecules' (Aueur, P.L. ed.), Gordon and Breach

Koenig, S.H. (1975)

Biopolymers 14, 2421

Kratky, O., Leopold, H. and Stabinger, H. (1969)

Z. Angew. Phys. 27, 273

Kratky, O., Leopold, H. and Stabinger, H. (1969)

in 'Methods in Enzymology' (Hirs, C.H.W. and Timasheff, S.N. eds.), 27, 98, Academic, London

Krause, S. and O'Konski, C.T. (1959)

J. Am. Chem. Soc. 81, 5082

Kuff, E.J. and Dalton, A.L. (1957)

J. Ultrastructure Res. 1, 62

Kuhn, W. and Kuhn, H. (1945)

Helvetica Chimica Acta 38, 97

Kynch, G.J. (1956)

Proc. Roy. Soc. (London) A237, 90

Labaw, L.W. and Wycoff, R.W.G. (1957)

Biochim. Biophys. Acta 25, 263

Lauffer, M.A. (1942)

Chem. Rev. 31, 561

Laurent, T.C. and Killander, J. (1964)

J. Chromatog. 14, 317

Lipscomb, W.N. (1971)

Proc. Robert A. Welch Found. Conf. Chem. Res. 15, 134

Lloyd, P.H. (1974)

'Optical Methods in Ultracentrifugation, Electrophoresis and Diffusion',

Clarendon Press, Oxford

Lucas, C.W. and Terrill, C.W. (1970)

Collected Algorithms from CACM, No. 404

Manley, R. and Mason, S. G. (1954)

Canad. J. Chem. 32, 763

Martin, R.B. (1964)

'Introduction to Biophysical Chemistry' Chap. 11, McGraw-Hill, New York

McCammon, J.A., Deutch, J.M. and Bloomfield, V.A. (1975)

Biopolymers 14, 2479

Mehl, J.W., Oncley, J.L. and Simha, R. (1940)

Science 92, 132

Mendelson, R. and Hartt, J. (1980)

EMBO Workshop on Muscle Contraction, Alpbach Conf. Austria

Mihalyi, E. and Godfrey, J. (1963)

Biochim. Biophys. Acta 67, 90

Memming, R. (1961)

Z. Physik. Chem. (Frankfurt) 28, 169

Mooney, M. (1951)

J. Coll. Sci. 6, 162

Mooney, M. (1957)

J. Coll. Sci. 12, 575

Munro, I., Pecht, I. and Stryer, L. (1979)

Proc. Nat. Acad. Sci. (USA) 76, 56

Nichol, L.W., Jeffrey, P.D., Turner, D.R. and Winzor, D.J. (1977)

J. Phys. Chem. 81, 776

Nisihara, T. and Doty, P. (1958)

Proc. Nat. Acad. Sci. (USA) 44, 411

Oberbeck, A. (1876)

J. reine. angew. Math. 81, 62

O'Connor, D.V., Ware, W.R. and Andre, J.C. (1979)

J. Phys. Chem. 83, 1333

Offer, G., Moos, C. and Starr, R. (1973)

J. Mol. Biol. 74, 653

O'Hara and Smith (1968)

Comp. Journal 11, 213

O'Konski, C.T. and Haltner, A.J. (1956)

J. Am. Chem. Soc. 78, 3604

Oliver, J. (1972)

Comp. Journal 15, 141

Oncley, J.L. (1940)

J. Phys. Chem. 44, 1103

Oncley, J.L. (1941)

Ann. New York Acad. Sci. 41, 121

Paradine, C.G. and Rivett, B.H.P. (1960)

'Statistical Methods for Technologists', English Universities Press, London

Pearce, T.C., Rowe, A.J. and Turnock, G. (1975)

J. Mol. Biol. 97, 193

Perrin, F. (1934)

J. Phys. Radium 5, 497

Perrin, F. (1936)

J. Phys. Radium 7, 1

Perutz, M.F., Rossmann, M.G., Cullis, A.F., Muirhead, H., Will, G. and North, A.C.T. (1960)

Nature 185, 416

Powell, D.R. and MacDonald, J.R. (1972)

Comp. Journal 15, 148

Pytkowickz, R.M. and O'Konski, C.T. (1959)

J. Am. Chem. Soc. 81, 5082

Rallison, J.M. (1978)

J. Fluid Mech. 84, 237

Riddiford, C.L. and Jennings, B.R. (1967)

Biopolymers 5, 757

Ridgeway, D. (1966)

J. Am. Chem. Soc. 88, 1104

Ridgeway, D. (1968)

J. Am. Chem. Soc. 90, 18

Rowe, A.J. (1977)

Biopolymers 16, 2595

Rowe, A.J. (1978)

Techniques in Protein and Enzyme Biochem. B105a, 1

Saito, N. (1951)

J. Phys. Soc. (Japan) 6, 297

Scheraga, H.A. (1955)

J. Chem. Phys. 23, 1526

Scheraga, H.A. (1961)

'Protein Structure', Academic, New York

Scheraga, H.A. and Mandelkern, L. (1953)

J. Am. Chem. Soc. 79, 179

Simha, R. (1940)

J. Phys. Chem. 44, 25

Simha, R. (1952)

J. Appl. Phys. 23, 1020

Shaw, D.J. (1970)

'Introduction to Colloid and Surface Chemistry' (2nd edn.), Butterworths

Small, E.W. and Isenberg, I. (1977)

Biopolymers 16, 1907

Sorenson, N.A. (1930)

CR Lab. Carlsberg 18, No. 5

Squire, P.G. (1970)

Biochim. Biophys. Acta 221, 425

Squire, P.G. (1978)

in 'Molecular Electro Optics' (O'Konski, C.T. ed.) Volume 2, 565

Squire, P.G., Moser, L. and O'Konski, C.T. (1968)

Biochemistry 7, 4261

Stacey, K.A. (1956)

'Light Scattering in Physical Chemistry', Butterworths, London

Stokes, Sir G. (1851)

Trans. Cambridge Phil. Soc. 9, 8

Stokes, Sir G. (1880)

'Mathematical and Physical Papers', Cambridge University Press

Svedberg, T. and Pedersen, K.O. (1940)

'The Ultracentrifuge', Oxford University Press

Tanford, C. (1955)

J. Phys. Chem. 59, 798

Tanford, C. (1961)

'Physical Chemistry of Macromolecules', Wiley, New York

Theorell, H. (1934)

Biochem. Z. 268, 46

Vand, V. (1948)

J. Phys. Coll. Chem. 52, 277

Van de Hulst, H.C. (1957)

'Light Scattering by Small Particles', Wiley, New York

Van Holde, K.E. (1971)

'Physical Biochemistry', Prentice Hall, New Jersey

Wahl, P. (1966)

Compt. Rend. Acad. Sci. (Paris) 263D 1525

Wales, M. and Van Holde, K.E. (1954)

J. Polymer Sci. 14, 81

Wilde, D.J. (1964)

'Optimum Seeking Methods', Prentice Hall, New Jersey

Williams, R.C., Ham, W.T. and Wright, A.K. (1976)

Anal. Biochem. 73, 52

Wilson, R.W. and Bloomfield, V.A. (1979a)

Biopolymers 18, 1205

Wilson, R.W. and Bloomfield, V.A. (1979b)

Biopolymers 18, 1543

Yang, J.T. (1961)

Adv. Protein Chem. 16, 323

Zimm, B.H. (1948)

J. Chem. Phys. 16, 1093

Zimm, B.H. (1956)

J. Chem. Phys. 24, 269