ANALYTICAL CALCULATION OF THE RADIUS OF GYRATION OF POLYHEDRA AND PLATONIC SOLIDS IN SMALL-ANGLE SCATTERING

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The radius of gyration (Rg) is one of the most important parameter to be extracted from small-angle scattering (SAXS, SANS) measurements of nanoparticles and contains information about size, shape, symmetry and homogeneity in one parameter. The analytical expressions for Rg are well known for simple geometrical shapes (spheres, ellipsoids, cylinders, cubes). In this work, the analytical equations for Rg for also other homogeneous (constant electron or scattering length density) shapes like cones, pyramids, paraboloids, hemispheres or tori are derived and are compiled in this poster. In this approach, the Rg of different 3-dimensional objects can be composed of a cross-sectional (Rc) and of a perpendicular contribution. Thus, Rg^2 is the linear sum of both, $Rg^2 = f_1 * Rc^2 + f_2 * h^2$, with h being the height or diameter of the object in the perpendicular direction to the cross-section and f_1 and f_2 being multiplicative factors with values depending on the geometrical shape. The cross-sectional area can be (semi-)circular, (semi-) elliptic, n-polygonal or rhombic, resulting in a conical, pyramidal, elliptic or parabolic 3D-shape, depending on the perpendicular component. A mirror-symmetry in the cross-sectional plane may be present (e.g. ellipsoids, bi-cones or bi-pyramids) or absent (e.g. hemispheres or single cones or pyramids). General equations of Rc for regular (equilateral) n-polygons will be given, but also for non-equilateral polygonal (rectangular, triangular) and rhombic cross-sections.

Furthermore, the analytical equations of Rg for the five Platonic polyhedra (tetrahedron, hexa-hedron, octahedron, dodecahedron and icosahedron) are presented, for the solid, for the hollow (faces only) and as well as for the skeletal (edges only) shape. The existence of such shapes in the nanoscale range has been demonstrated for instance by He et al. [1] and can be constructed by hierarchical self-assembly of DNA into symmetric supramolecular polyhedral nanostructures. Recently, also the small-angle scattering functions in reciprocal and real space of Platonic solids have been derived by Li et al. [2].

[1] Y.He, T.Ye, M.Su, C.Zhang, A.E.Ribbe, W.Jiang and C.Mao, *Nature*, **452**, 198-201 (2008).

[2] X.Li, C.-Y.Shew, L.He, F.Meilleur, D.A.A.Myles, E.Liu, Y.Zhang, G.S.Smith, K.W.Herwig, R.Pynn and W.-R.Chen, *J.Appl.Cryst.*, **44**, 545-557 (2011).