Analytical calculation of the radius of gyration of regular shapes and polyhedra

M. Kriechbaum

Graz University of Technology, Institute of Inorganic Chemistry, Graz, Austria

The radius of gyration (Rg) is one of the most common parameters to be extracted from small-angle X-ray/neutron scattering (SAXS, SANS) measurements of nanoparticles and combines information about size, shape, symmetry and homogeneity in one single value. The analytical expressions for Rg are well known for simple geometric shapes (spheres, ellipsoids, cylinders, cubes). In this work, the analytical equations for Rg for 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 2-dimensional cross-sectional (Rc) and of a perpendicular (h) contribution. Thus, \( R_g^2 = f_1 R_c^2 + f_2 h^2 \), 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 geometric shape. The cross-sectional area can be (semi-)circular, (semi-)elliptic, n-polygonal or rhombic, resulting in a conical, pyramidal, ellipsoidal or paraboloidal 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 of nanoscaled particles of high symmetry, in particular of convex polyhedra like the 5 Platonic solids (tetra-, hexa-, octa-, dodeca- and icosahedron) or the 13 Archimedean solids and their duals (Catalan solids) are presented, for the solid, for the hollow (faces only) and as well as for the skeletal (edges only) and dot (vertices only) shape.

Keywords: radius of gyration, small angle scattering, polyhedral shape