ANALYTICAL CALCULATION OF THE RADIUS OF GYRATION OF REGULAR SHAPES AND POLYHEDRA

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Introduction

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, Rg^2 is the linear sum of both: $Rg^2 = f1*Rc^2 + f2*h^2$, with h being the height or diameter of the object in the perpendicular direction to the cross-section and f1 and f2 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 icosa-hedron) 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.

Polyhedra, Pyramids, Cylinders, Ellipsoids, Cones and Tori

Master equation:: $$Rg^2 = f_1 * Rc^2 + f_2 * h^2 \quad (1)$$

with:

n-Polygon: $$Rc^2 = \frac{1}{8} * \left(\frac{1}{t^2} + \frac{1}{3}\right) * a^2 = \frac{1}{8} * \left(\frac{1}{s^2} - \frac{2}{3}\right) * a^2 \quad (2a)$$

Circle: $$Rc^2 = \frac{1}{2} * r^2 \quad (2b)$$

Rg: Radius of gyration of the entire solid (3D) shape
Rc: cross-sectional (2D) Radius of gyration
a: edge length of (equilateral) n-polygon
r: radius of circle
$t = tan(\pi/n)$ and $s = sin(\pi/n)$
n: number of vertices of an n-polygon (>2)
h: height (cone/pyramid) or diameter (ellipsoid/paraboloid) in direction of z-axis (normal to the plane of cross-section) or radial diameter of the circular torus in the xy-plane (2 x R_T), respectively.

Shape (solid)	Volume	Centroid (Mono)	f_1	f_2 (Mono)	f_2 (Bi-)	f_2 (Double-)
Cylinder/Prism	$area * h$	$1/2 * h$	1	1/12	1/12	1/12
(Semi-)Ellipsoid	$area * 2h/3$	$3/8 * h$	4/5	19/320	1/20	9/80
Paraboloid	$area * h/2$	$1/3 * h$	2/3	1/18	1/24	1/8
Cone/Pyramid	$area * h/3$	$1/4 * h$	3/5	3/80	1/40	3/20
Torus	$area * \pi * h$	$1/2 * h$	2	1/4	–	–

Shape (shell)	Area	Centroid (Mono)	f_1	f_2 (Mono)	f_2 (Bi-)	f_2 (Double-)
Cylinder/Prism	$cf * h$	$1/2 * h$	1	1/12	1/12	1/12
(Semi-)Ellipsoid	$cf * h$	$1/2 * h$	2/3	1/12	1/12	1/12
Cone/Pyramid	$cf * \pi * s/2$	$1/3 * h$	1/2	1/18	1/24	1/8
Torus	$cf * \pi * h$	$1/2 * h$	4	1/4	–	–

$Rc^2\ (shell) = 2 * Rc^2\ (solid)$; cf: circumference, s: lateral height

Tab.1: Volume/area (calculated from the cross-sectional area/cf and height or diameter h), centroid and multiplicative factors f_1 and f_2 used for the calculation of the radius of gyration Rg (equ.1) for various shapes (solids and shells). The term "mono" indicates the shape with the base (cross-section) centered at $z = 0$ and with height h, extending in the z-direction (perpendicular to the base, from $z = 0$ to $z = h$) and the centroid of the solid/shell is located at a fraction of h as given in the table. This refers to a pyramid or cone, to a solid/shell paraboloid or solid/shell semi-ellipsoid. The terms "Bi-" and "Double-", respectively, refer to shapes where the solids/shells are attached symmetrically at a mirror-plane which is either the cross-section ("Bi-") or the apex ("Double-") of the solid/shell, resulting in a bi- or double-cone/paraboloid or ellipsoid with total height or diameter h in the z-direction. The shape's centroid in these cases would be at $z = h/2$ (location of the mirror-plane). The z-axis (perpendicular to the cross-section) passes through the cross-sectional centroid and the apex.
In case of a torus h is the diameter of the torus-ring (the ring passes through the centroid of the tubular cross-section and the centroid of the entire torus is located at the origin of the torus radius ($h/2$).

Shape of cross-section	Rc^2	remark
g-Triangle	$\frac{1}{36} * a^2 + \frac{1}{36} * b^2 + \frac{1}{36} * c^2$	general triangle: sides: a, b, c
r-Triangle	$\frac{1}{18} * a^2 + \frac{1}{18} * b^2$	right triangle: sides: $a \perp b$
i-Triangle	$\frac{1}{18} * a^2 + \frac{1}{36} * b^2$	isosceles triangle: sides: a, a, b
Rectangle	$\frac{1}{12} * a^2 + \frac{1}{12} * b^2$	
Rhombus	$\frac{1}{6} * ra^2 + \frac{1}{6} * rb^2$	
Ellipse	$\frac{1}{4} * ra^2 + \frac{1}{4} * rb^2$	
Semi-ellipse	$\left(\frac{1}{4} - k^2\right) * ra^2 + \frac{1}{4} * rb^2$	ellipse is cut along rb
Quarter-ellipse	$\left(\frac{1}{4} - k^2\right) * ra^2 + \left(\frac{1}{4} - k^2\right) * rb^2$	

$a, b, (c)$: edge lengths of the rectangle (triangle), ra, rb: semi-axes of the rhombus or ellipse, respectively and $k = 4/(3 * \pi)$.

Tab.2: These equations for Rc (squared) can be used in equ. (1) for Rg-calculations for prisms, cones, pyramids and tori. For tori the weighting factors for ra and rb for calculating Rc (equ. 2b) are *3/8* and *1/8*, respectively, with ra parallel to the torus-plane and rb parallel to the torus z-axis.

Platonic Solids / Archimedean Solids / Catalan Solids

shape	$Rg_s^2 = c * a^2$ solids	$Rg_f^2 = c * a^2$ faces	$Rg_e^2 = c * a^2$ edges	$Rg_v^2 = c * a^2$ vertices
T	$3/40$	$1/8$	$5/24$	$3/8$
H	$1/4$	$5/12$	$7/12$	$3/4$
O	$3/20$	$1/4$	$1/3$	$1/2$
D	$(95 + 39 * \sqrt{5})/200$	$(95 + 39 * \sqrt{5})/120$	$(23 + 9 * \sqrt{5})/24$	$(9 + \sqrt{45})/8$
I	$(9 + 3 * \sqrt{5})/40$	$(3 + \sqrt{5})/8$	$(11 + 3 * \sqrt{5})/24$	$(5 + \sqrt{5})/8$

Tab.3: Multiplicative factor c used for the calculation of the radius of gyration Rg (squared) of Platonic Solids, Shells (Faces), Skeletons and Dots (Vertices) solely as a function of one parameter, the edge length a.

Type of Platonic Shape	Equation for Rg^2
Platonic Solids:	$3/5 * (Rc^2 + ri^2)$
Platonic "Shells" (faces only):	$Rc^2 + ri^2$
Platonic "Skeletons" (edges only):	$(1/12 * a^2) + rm^2$
Platonic "Dots" (vertices only):	rc^2

Tab.4: In these equs. ri, rm, rc are the radii of the in-sphere, mid-sphere and circum-sphere of the respective Platonic solid which can be calculated as a function of edge length a [3]. The parameter Rc is the cross-sectional Radius of gyration of the respective polygonal face which the Platonic Solids consist of. Rc can be computed by equ. (2), using a triangle for the Tetra-, Octa- and Icosahedron (T, O, I), a square for the Hexahedron (H) and a pentagon for the Dodecahedron (D), respectively, with (equilateral) edge lengths a.

Archimedean Solid	Rg(s)	Rg(f)	Rg(e)	Rg(v)	f	e	v	Rg(v)	Rg(e)	Rg(f)	Rg(s)	Dual
Truncated Tetrahedron	0.51643	0.65705	0.78839	0.84100	8	18	12	0.84671	0.75184	0.65299	0.50581	Triakis Tetrahedron
Truncated Octahedron	0.48542	0.62564	0.68044	0.70432	14	36	24	0.71487	0.66002	0.62412	0.48344	Tetrakis Hexahedron
Truncated Cube	0.49486	0.63546	0.72534	0.74523	14	36	24	0.71843	0.68337	0.63082	0.48863	Triakis Octahedron
Truncated Icosahedron	0.48105	0.62099	0.64158	0.65047	32	90	60	0.65772	0.63364	0.62077	0.48085	Pentakis Dodecahedron
Truncated Dodecahedron	0.48362	0.62373	0.66884	0.67526	32	90	60	0.65267	0.64373	0.62229	0.48203	Triakis Icosahedron
Cuboctahedron	0.48697	0.62740	0.68594	0.75141	14	24	12	0.73482	0.68736	0.62748	0.48604	Rhombic Dodecahedron
Icosidodecahedron	0.48231	0.62212	0.65219	0.67399	32	60	30	0.66228	0.64641	0.62176	0.48161	Rhombic Triacontahedron
Snub Cube	0.48151	0.62142	0.64307	0.67498	38	60	24	0.66308	0.64913	0.62161	0.48150	Pentagonal Icositetrahedron
Snub Dodecahedron	0.48088	0.62066	0.63177	0.64341	92	150	60	0.63613	0.63208	0.62062	0.48073	Pentagonal Hexecontahedron
Small Rhombicuboctah.	0.48173	0.62180	0.65024	0.67983	26	48	24	0.67536	0.65001	0.62176	0.48161	Deltoidal Icositetrahedron
Great Rhombicuboctah.	0.48308	0.62273	0.65737	0.66781	26	72	48	0.66544	0.64201	0.62193	0.48174	Disdyakis Dodecahedron
Small Rhombicosidodecah.	0.48081	0.62066	0.63350	0.64436	62	120	60	0.64153	0.63206	0.62061	0.48072	Deltoidal Hexecontahedron
Great Rhombicosidodecah.	0.48137	0.62107	0.63927	0.64299	62	180	120	0.63669	0.62992	0.62077	0.48085	Disdyakis Triacontahedron
Dual	Rg(s)	Rg(f)	Rg(e)	Rg(v)	v	e	f	Rg(v)	Rg(e)	Rg(f)	Rg(s)	Catalan Solid
Sphere	0.48052	0.62035	0.62035	0.62035	0	0	0	0.62035	0.62035	0.62035	0.48052	Sphere

Tab.5: The values for the Radius of Gyration of the solid (Rgs), of the faces (Rgf), of the edges (Rge) and of the vertices (Rgv) of the 13 Archimedean Solids and their corresponding Duals, the Catalan Solids, all with their respective volume normalized to V=1, are compiled together with the number of the faces (f), edges (e) and vertices (v) for each polyhedron. All these polyhedra can be decomposed into pyramids with n-polygonal bases. For comparison, also the Rg-values for a sphere with the same volume (V=1) are given. Units are arbitrary.

RG-calculator on the Web:
http://www.staff.tugraz.at/manfred.kriechbaum/xitami/java/rgpoly.html
http://www.staff.tugraz.at/manfred.kriechbaum/xitami/java/rgplaton.html
http://www.staff.tugraz.at/manfred.kriechbaum/xitami/java/rgpolyhedra.html
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