A Practical Guide to Calculate the Number of Atoms and Overall Composition of Metal Nanoparticles using Geometric Considerations

Taizo Mori*[#] and Torsten Hegmann*

Chemical Physics Interdisciplinary Program, Liquid Crystal Institute, Kent State University, Kent, OH 44242-0001 U.S.A.

Electronic Supplementary Material

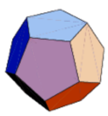
Section S1 – Equations and calculations for Platonic, Archimedean and Catalan solids[S1]

Platonic Solids

Icosahedron
Vertices: 12
Faces: 20 [3]
Edges: 30
Dual solid: Dodecahedron

$$V = \frac{5(3+\sqrt{5})}{12}L^3 = 2.182L^3 \qquad S = 5\sqrt{3}L^2 = 8.660L^2$$

$$R_c = \frac{\sqrt{10+2\sqrt{5}}}{4}L = 0.9511L \qquad R_m = \frac{1+\sqrt{5}}{4}L = 0.8090L \qquad R_i = \frac{3\sqrt{3}+\sqrt{15}}{12}L = 0.7558L$$



Dodecahedron
Vertices: 20
Faces: 12 [5]
Edges: 30
Dual solid: Icosahedron

$$V = \frac{15+7\sqrt{5}}{4}L^3 = 7.663L^3 \qquad S = 3\sqrt{25+10\sqrt{5}}L^2 = 20.65L^2$$

$$R_c = \frac{\sqrt{3}+\sqrt{15}}{4}L = 1.4013L \qquad R_m = \frac{3+\sqrt{5}}{4}L = 1.3090L \qquad R_i = \frac{\sqrt{10(25+11\sqrt{5})}}{20}L = 1.1135L$$

Archimedean Solids

Truncated Tetrahedron
Vertices: 12
Faces: 8 = 4[3] + 4[6]
Edges: 18
Dual solid: Triakis Tetrahedron

$$V = \frac{23}{12}\sqrt{2}L^3 = 2.711L^3 \qquad S = 7\sqrt{3}L^2 = 12.12L^2$$

$$R_c = \frac{\sqrt{22}}{4}L = 1.1726L \qquad R_m = \frac{3\sqrt{2}}{4}L = 1.0606L$$

[3]: $R_i = \frac{5\sqrt{6}}{12}L = 1.0206L$
[6]: $R_i = \frac{\sqrt{6}}{4}L = 0.6123L$

Cuboctahedron
Vertices: 12
Faces: 14 = 8[3] + 6[4]
Edges: 24
Dual solid: Rhombic Dodecahedron

$$V = \frac{5}{3}\sqrt{2}L^3 = 2.357L^3 \qquad S = (6+2\sqrt{3})L^2 = 9.464L^2$$

$$R_c = L \qquad R_m = \frac{\sqrt{3}}{2}L = 0.8660L$$

[3]: $R_i = \frac{\sqrt{6}}{3}L = 0.8165L$
[4]: $R_i = \frac{\sqrt{2}}{2}L = 0.7071L$

Truncated Octahedron
Vertices: 24
Faces: 14 = 6[4] + 8[6]
Edges: 36
Dual solid: Tetrakis Hexahedron

$$V = 8\sqrt{2}L^3 = 11.31L^3 \qquad S = 6(1+2\sqrt{3})L^2 = 26.78L^2$$

$$R_c = \frac{\sqrt{10}}{2}L = 1.5811L \qquad R_m = 1.5L$$

[4]: $R_i = \sqrt{2}L = 1.4142L$
[6]: $R_i = \frac{\sqrt{6}}{2}L = 1.2247L$

V: *Volume*, S: *Surface area*, L: *Edge length*, R_c: *Circumscribed radius*, R_m: *Midscribed radius*, R_i: *Inscribed radius*

Truncated Cube
Vertices: 24
Faces: 14 = 8[3] + 6[8]
Edges: 36
Dual solid: Triakis Octahedron

$$V = 7\left(1+\frac{2\sqrt{2}}{3}\right)L^3 = 13.56L^3 \qquad S = 2\left(6+6\sqrt{2}+\sqrt{3}\right)L^2 = 32.43L^2$$

$$R_c = \frac{\sqrt{7+4\sqrt{2}}}{2}L = 1.7789L \qquad R_m = \left(1+\frac{\sqrt{2}}{2}\right)L = 1.7071L$$

$$[3]:\ R_i = \frac{3\sqrt{3}+2\sqrt{6}}{6}L = 1.6825L$$

$$[8]:\ R_i = \frac{1+\sqrt{2}}{2}L = 1.2071L$$

Rhombicuboctahedron
Vertices: 24
Faces: 26 = 8[3] + 18[4]
Edges: 48
Dual solid: Deltoidal Icositetrahedron

$$V = \frac{2}{3}\left(6+5\sqrt{2}\right)L^3 = 8.7140L^3 \qquad S = \left(18+2\sqrt{3}\right)L^2 = 21.46L^2$$

$$R_c = \frac{\sqrt{5+2\sqrt{2}}}{2}L = 1.3990L \qquad R_m = \frac{\sqrt{2\left(2+\sqrt{2}\right)}}{2}L = 1.3066L$$

$$[3]:\ R_i = \frac{3\sqrt{3}+\sqrt{6}}{6}L = 1.2743L$$

$$[4]:\ R_i = \frac{1+\sqrt{2}}{2}L = 1.2071L$$

Snub Cube (enantiomer)
Vertices: 24
Faces: 38 = 32[3] + 6[4]
Edges: 60
Dual solid: Pentagonal Icositetrahedron

$$V = \frac{3\sqrt{\tau-1}+4\sqrt{\tau+1}}{3\sqrt{2-\tau}}L^3 = 7.8895L^3 \qquad S = \left(6+8\sqrt{3}\right)L^2 = 18.86L^2$$

$$R_c = \frac{\sqrt{d^2+L^2}}{2} = 1.3437L \qquad R_m = \frac{1}{\sqrt{4(2-\tau)}}L = 1.2472L$$

$$[3]:\ R_i = \frac{\sqrt{d^2-L^2}}{2} = 1.2134L$$

$$\tau = \left(X^3-X^2-X-1\right)_1 = \frac{1}{3}\left(1+\sqrt[3]{19-2\sqrt{33}}+\sqrt[3]{19+2\sqrt{33}}\right) = 1.83929$$

$$d = \frac{L}{\sqrt{2-\tau}}$$

$$[4]:\ R_i = \frac{1}{2}\sqrt{d^2-\frac{L^2}{3}} = 1.1426L$$

Truncated Cuboctahedron
Vertices: 48 (48[3])
Faces: 26 = 12[4] + 8[6] +6[8]
Edges: 72
Dual solid: Disdyakis Dodecahedron

$$V = \left(22+14\sqrt{2}\right)L^3 = 41.79L^3 \qquad S = 12\left(2+\sqrt{2}+\sqrt{3}\right)L^2 = 61.76L^2$$

$$R_c = \frac{\sqrt{13+6\sqrt{2}}}{2}L = 2.3176L \qquad R_m = \frac{\sqrt{12+6\sqrt{2}}}{2}L = 2.2630L$$

$$[4]:\ R_i = \frac{3+\sqrt{2}}{2} = 2.2071L$$

$$[6]:\ R_i = \frac{\sqrt{3}+\sqrt{6}}{2} = 2.0908L$$

$$[8]:\ R_i = \frac{1+2\sqrt{2}}{2} = 1.9142L$$

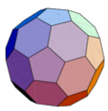
Icosidodecahedron
Vertices: 30
Faces: 32 = 20[3] + 12[5]
Edges: 60
Dual solid: Rhombic Triacontahedron

$$V=\frac{45+17\sqrt{5}}{6}L^3=13.84L^3 \qquad S=\left(5\sqrt{3}+3\sqrt{5}\sqrt{5+2\sqrt{5}}\right)L^2=29.31L^2$$

$$R_c=\frac{1+\sqrt{5}}{2}L=1.6180L \qquad R_m=\frac{\sqrt{5+2\sqrt{5}}}{2}L=1.5388L$$

$$[3]:\ R_{in}=\sqrt{\frac{7+3\sqrt{5}}{6}}=1.5115L$$

$$[5]:\ R_{in}=\sqrt{\frac{5+2\sqrt{5}}{5}}L=1.3764L$$



Truncated Icosahedron
Vertices: 60
Faces: 32 = 12[5] + 20[6]
Edges: 90
Dual solid: Pentakis Dodecahedron

$$V=\frac{125+43\sqrt{5}}{4}L^3=55.29L^3 \qquad S=3\left(10\sqrt{3}+\sqrt{5}\sqrt{5+2\sqrt{5}}\right)L^2=72.61L^2$$

$$R_c=\frac{\sqrt{58+18\sqrt{5}}}{4}L=2.4780L \qquad R_m=\frac{3(1+\sqrt{5})}{4}L=2.4271L$$

$$[5]:\ R_i=\frac{\sqrt{10(125+41\sqrt{5})}}{20}=2.3274L$$

$$[6]:\ R_i=\frac{3\sqrt{5}+\sqrt{15}}{4}=2.2672L$$

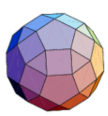
Truncated Dodecahedron
Vertices: 60
Faces: 32 = 20[3] + 12[10]
Edges: 90
Dual solid: Triakis Icosahedron

$$V=\frac{5}{12}(99+47\sqrt{5})L^3=85.04L^3 \qquad S=5\left(\sqrt{3}+6\sqrt{5+2\sqrt{5}}\right)L^2=100.99L^2$$

$$R_c=\frac{\sqrt{2(37+15\sqrt{5})}}{4}L=2.9695L \qquad R_m=\frac{5+3\sqrt{5}}{4}L=2.9271L$$

$$[3]:\ R_i=\frac{9\sqrt{3}+5\sqrt{15}}{12}=2.9128L$$

$$[10]:\ R_i=\frac{\sqrt{2(25+11\sqrt{5})}}{4}L=2.499L$$



Rhombicosidodecahedron
Vertices: 60
Faces: 62 = 20[3] + 30[4] + 12[5]
Edges: 120
Dual solid: Deltoidal Hexecontahedron

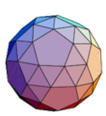
$$V=\left(20+\frac{29}{3}\sqrt{5}\right)L^3=41.62L^3 \qquad S=\left\{30+\sqrt{30\left[10+3\sqrt{5}+\sqrt{15(5+2\sqrt{5})}\right]}\right\}L^2=59.31L^2$$

$$R_c=\frac{\sqrt{11+4\sqrt{5}}}{2}L=2.2330L \qquad R_m=\frac{\sqrt{2(5+2\sqrt{5})}}{2}L=2.1763L$$

$$[3]:\ R_i=\frac{3\sqrt{3}+2\sqrt{15}}{6}=2.1571L$$

$$[4]:\ R_i=\frac{2+\sqrt{5}}{2}=2.1180L$$

$$[5]:\ R_i=\frac{3\sqrt{5(5+2\sqrt{5})}}{10}=2.0653L$$



Snub Dodecahedron (enantiomer)
Vertices: 60
Faces: 92 = 80[3] + 12[5]
Edges: 150
Dual solid: Pentagonal Hexecontahedron

$$\phi=\frac{1+\sqrt{5}}{2} \qquad \xi=\sqrt[3]{\frac{\phi+\sqrt{\phi-5/27}}{2}}+\sqrt[3]{\frac{\phi-\sqrt{\phi-5/27}}{2}}$$

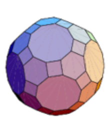
$$V=\frac{12\xi^2(3\phi+1)-\xi(36\phi+7)-(53\phi+6)}{6\sqrt{6-\xi^2}^3}=37.62L^3 \qquad S=20\sqrt{3}+3\sqrt{25+10\sqrt{5}}=55.289$$

$$R_c=\phi\sqrt{\xi(\xi+\phi)}+\frac{3-\phi}{2}=2.1558L$$

$$R_m=\frac{\phi\sqrt{\xi(\xi+\phi)+1}}{2}L=2.0971L$$

$$[3]:\ R_i=\frac{\phi\xi\sqrt{3[\xi(\xi+\phi)+1]}}{6}=2.0771L$$

$$[5]:\ R_i=\sqrt{20\left[5\left(\xi+\frac{1}{\xi}\right)(2\phi+1)\right]+\frac{11\phi+12}{20}}=1.9809L$$



Truncated Icosidodecahedron
Vertices: 120
Faces: 62 = 30[4] + 20[6] + 12[12])
Edges: 180
Dual solid: Disdyakis Triacontahedron

$$V=(95+50\sqrt{5})L^3=206.80L^3 \qquad S=30\left(1+\sqrt{2\left(4+\sqrt{5}+\sqrt{15+6\sqrt{6}}\right)}\right)L^2=175.03L^2$$

$$R_c=\frac{\sqrt{31+12\sqrt{5}}}{2}L=3.8024L$$

$$R_m=\frac{\sqrt{6(5+2\sqrt{2})}}{2}L=3.7694L$$

$$[4]:\ R_i=\frac{3+2\sqrt{5}}{2}=3.7361L$$

$$[6]:\ R_i=\frac{2\sqrt{3}+\sqrt{15}}{2}=3.6685L$$

$$[12]:\ R_i=\frac{\sqrt{5(5+2\sqrt{5})}}{2}=3.4410L$$

Catalan Solids

Triakis Tetrahedron

]ertices: 8
Faces: 12 (isosceles triangles)
Edges: 18 = $12L_s + 6L_l$
Dual solid: Truncated Tetrahedron

$V = \frac{8\sqrt{2}}{20}a^3 = 5.7276a^3$ $\quad S = \frac{27}{5}\sqrt{11}a^2 = 17.91$ $\quad L_s = \frac{9}{5}a = 1.8a$, $L_l = 3a$

[3]: $R_v = \frac{9\sqrt{6}}{20}a = 1.1023a$ $\quad R_e = \frac{3\sqrt{2}}{3}a = 1.0607a$ $\quad R_i = \frac{9\sqrt{22}}{44}a = 0.9594a$

[6]: $R_v = \frac{3\sqrt{6}}{4}a = 1.8371a$

Rhombic Dodecahedron

Vertices: 14
Faces: 12 (rhombi)
Edges: 24
Dual solid: Cuboctahedron

$V = \frac{27\sqrt{2}}{16}a^3 = 2.3865a^3$ $\quad S = \frac{4\sqrt{2}}{27}a^2 = 9.5460a^2$ $\quad L = \frac{3\sqrt{6}}{8}a = 0.9186a$

[3]: $R_v = \frac{3\sqrt{6}}{8}a = 0.9186a$ $\quad R_e = \frac{2\sqrt{2}}{3}a = 0.9428a$ $\quad R_i = \frac{3}{4}a = 0.75a$

[4]: $R_v = \frac{3\sqrt{2}}{4}a = 1.0607a$

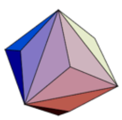
Tetrakis Hexahedron

Vertices: 14
Faces: 24 (isosceles triangles)
Edges: 36 = $24L_s + 12L_l$
Dual solid: Truncated Octahedron

$V = \frac{81\sqrt{2}}{8}a^3 = 14.32a^3$ $\quad S = \frac{27\sqrt{5}}{2}a^2 = 30.19a^2$ $\quad L_s = \frac{9\sqrt{2}}{8}a = 1.5910a$, $L_l = \frac{3\sqrt{2}}{2}a = 2.1213a$

[4]: $R_v = \frac{9\sqrt{2}}{8}a = 1.5910a$ $\quad R_e = \frac{3}{2}a = 1.5a$ $\quad R_i = \frac{9\sqrt{10}}{20}a = 1.423a$

[6]: $R_v = \frac{3\sqrt{6}}{4}a = 1.8371a$



Triakis Octahedron

Vertices: 14
Faces: 24 (isosceles triangles)
Edges: 36 = $24L_s + 12L_l$
Dual solid: Truncated Cube

$V = 4(3+\sqrt{2})a^3 = 23.31a^3$ $\quad S = 12\sqrt{7+4\sqrt{2}}a^2 = 42.69a^2$ $\quad L_s = 2a$, $L_l = (2+\sqrt{2})a = 3.4142a$

[3]: $R_v = \sqrt{3}a = 1.7321a$
[8]: $R_v = (1+\sqrt{2})a = 2.4142a$

$R_e = 1 + \frac{\sqrt{2}}{2}a = 1.7072a$ $\quad R_i = \frac{\sqrt{17(23+16\sqrt{2})}}{17}a = 1.6383a$

Deltoidal Icositetrahedron

Vertices: 26
Faces: 24 (tri-equiangular kites)
Edges: 48 = $24L_s + 24L_l$
Dual solid: Rhombicuboctahedron

$V = \sqrt{122+71\sqrt{2}}L_s^3 = \frac{16(1+2\sqrt{2})}{7}a^3 = 8.7507a^3$ $\quad S = 6\sqrt{29-2\sqrt{2}}L_s^2 = 21.51a^2$ $\quad L_s = \frac{2\sqrt{10-\sqrt{2}}}{7}a = 0.8372a$, $L_l = \sqrt{2(2-\sqrt{2})}a = 1.0824a$

[3]: $R_v = \frac{4\sqrt{3}+\sqrt{6}}{7}a = 1.3397a$
[4]: $R_v = \sqrt{2}a = 1.4142a$

$R_e = \frac{\sqrt{2(2+\sqrt{2})}}{2}a = 1.3066a$ $\quad R_i = \frac{\sqrt{34(7+4\sqrt{2})}}{17}a = 1.2203a$

a: *Edge length of dual solid*, R_v: *Vertex radius*, R_e: *Edge − scribed radius*

Rhombic Triacontahedron

Vertices: 32
Faces: 30 (rhombi)
Edges: 60
Dual solid: Icosidodecahedron

$$V = 4\sqrt{5+2\sqrt{5}}L^3 = 12.31L^3 = \frac{25\sqrt{5+2\sqrt{5}}}{16}a^3 = 14.80a^3$$

$$S = 12\sqrt{5}L^2 = 26.84L^2 = 30.34a^2$$

$$L = \frac{\sqrt{10(5+\sqrt{5})}}{8}a = 1.0633\text{a}$$

$$[3]:\ R_{cs} = \frac{5\sqrt{3}+\sqrt{15}}{8}a = 1.5667a$$

$$[5]:\ R_{cs} = \frac{\sqrt{5(5+2\sqrt{5})}}{4}a = 1.7204a$$

$$R_e = \frac{\sqrt{5+2\sqrt{5}}}{2}a = 1.5388a$$

$$R_i = \frac{5+3\sqrt{5}}{8}a = 1.4635a$$

Pentagonal Icositetrahedron (enantiomer)

Vertices: 38
Faces: 24 (mirror-symmetric pentagons)
Edges: 60 = $36L_s + 24L_l$
Dual solid: Snub Cube

$$V = \sqrt{\frac{11(\tau-4)}{2(20\tau-37)}}a^3 = 7.4474a^3$$

$$S = 3\sqrt{\frac{22(5\tau-1)}{4\tau-3}}a^2 = 19.2999a^2$$

$$L_s = \frac{1}{\sqrt{\tau+1}}a = 0.593465a$$

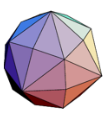
$$L_l = \frac{\sqrt{\tau+1}}{2}a = 1.0824a$$

$$[3]:\ R_v = \frac{\sqrt{2\left[6+\sqrt[3]{6(9+\sqrt{33})}+\sqrt[3]{6(9-\sqrt{33})}\right]}}{4}a = 1.2820L$$

$$[4]:\ R_v = \frac{\sqrt{6\left[14+\sqrt[3]{2(1777+33\sqrt{33})}+\sqrt[3]{2(1777-33\sqrt{33})}\right]}}{12}a = 1.3614a$$

$$R_e = \frac{\sqrt{3\left[7+\sqrt[3]{199+3\sqrt{33}}+\sqrt[3]{199-3\sqrt{33}}\right]}}{6}a = 1.2472a$$

$$R_i = \frac{\sqrt{42\left[78+\sqrt[3]{66(6039+49\sqrt{33})}+\sqrt[3]{66(6039-49\sqrt{33})}\right]}}{84}a = 1.1577a$$



Disdyakis Dodecahedron

Vertices: 26
Faces: 48 (acute triangles)
Edges: 72 = $24L_s + 24L_{lm} + 24L_l$
Dual solid: Truncated Cuboctahedron

$$V = \frac{144(1+\sqrt{2})}{7}a^3 = 49.6638a^3$$

$$S = \frac{6\sqrt{783+436\sqrt{2}}}{7}L_s^2 = 67.42a^2$$

$$L_s = \frac{2\sqrt{3(10-\sqrt{2})}}{7}a = 1.4500a$$

$$L_m = \frac{3\sqrt{6(2+\sqrt{2})}}{7}a = 1.9397a$$

$$L_l = \frac{2\sqrt{6(10+\sqrt{2})}}{7}a = 2.3644a$$

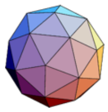
$$[4]:\ R_v = \frac{3(4+\sqrt{7})}{7}a = 2.3204a$$

$$[6]:\ R_v = \sqrt{6}a = 2.4495a$$

$$[8]:\ R_v = \frac{3(2+3\sqrt{2})}{7}a = 2.6754a$$

$$R_e = \frac{\sqrt{6(2+\sqrt{3})}}{2}a = 2.2630a$$

$$R_i = \frac{\sqrt{1746(15+8\sqrt{2})}}{97}a = 2.2097a$$



Pentakis Dodecahedron

Vertices: 32
Faces: 60 (isosceles triangles)
Edges: 90 = $60L_s + 30L_l$
Dual solid: Truncated Icosahedron

$$V = \frac{405(9+\sqrt{5})}{76}a^3 = \frac{5(41+25\sqrt{5})}{36}L_s^3 = 59.88a^3$$

$$L_s = \frac{9(2\sqrt{5}-1)}{19}a = 1.6447a$$

$$L_l = \frac{3(\sqrt{5}-1)}{2}a = 1.8541a$$

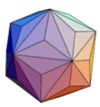
$$R_e = \frac{3\sqrt{1+\sqrt{5}}}{4}a = 2.4271a$$

$$S = \frac{5}{3}\sqrt{\frac{421+63\sqrt{5}}{2}}L_s^2 = 75.56a^2$$

[5]: $R_v = \frac{9\sqrt{65+22\sqrt{5}}}{38}a = 2.5309a$

[6]: $R_v = \frac{3\sqrt{3}}{2}a = 2.5981a$

$$R_i = \frac{9\sqrt{109(17+6\sqrt{5})}}{218}a = 2.3771a$$



Triakis Icosahedron

Vertices:
Faces: 60 (isosceles triangles)
Edges: 90 = $60L_s + 30L_l$
Dual solid: Truncated Dodecahedron

$$V = \frac{125(19+9\sqrt{5})}{44}a^3 = 111.15a^3$$

$$L_s = \frac{5(7+\sqrt{5})}{22}a = 2.0991a$$

$$L_l = \frac{5+\sqrt{5}}{2}a = 3.6180a$$

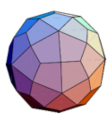
$$R_e = \frac{5+3\sqrt{5}}{4}a = 2.9271a$$

$$S = \frac{75}{11}\sqrt{\frac{313+117\sqrt{5}}{2}}a^2 = 115.57a^2$$

[3]: $R_v = \frac{5(3\sqrt{3}+2\sqrt{15})}{22}a = 2.9414a$

[10]: $R_v = \frac{\sqrt{5(5+2\sqrt{5})}}{2}a = 3.4410a$

$$R_i = \frac{5\sqrt{61(41+18\sqrt{5})}}{122}a = 2.8853a$$



Deltoidal Hexecontahedron

Vertices: 62
Faces: 60 (kites)
Edges: 120 = $60L_s + 60L_l$
Dual solid: Rhombicosidodecahedron

$$V = \frac{100(5+4\sqrt{5})}{33}a^3 = 42.26a^3$$

$$L_s = \frac{\sqrt{5(85-31\sqrt{5})}}{11}a = 0.8050a$$

$$L_l = \frac{\sqrt{5(5-\sqrt{5})}}{3}a = 1.2392a$$

$$R_e = \frac{\sqrt{2(5+2\sqrt{5})}}{2}a = 2.1763a$$

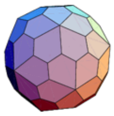
$$S = \frac{100}{11}\sqrt{79-16\sqrt{5}}a^2 = 59.77a^2$$

[3]: $R_v = \frac{5\sqrt{3}+4\sqrt{15}}{11}a = 2.1957a$

[4]: $R_v = \sqrt{5}a = 2.2361a$

[5]: $R_v = \frac{\sqrt{5(5+2\sqrt{5})}}{3}a = 2.2940a$

$$R_i = \frac{\sqrt{205(19+8\sqrt{5})}}{41}a = 2.1210a$$



Pentagonal Hexecontahedron (enantiomer)

Vertices: 92 (80[3] + 12[5])

Faces: 60 (mirror-symmetric pentagons)

Edges: 150 = $90L_s + 60L_l$

Dual solid: Snub Dodecahedron

$$L_s = \frac{1}{\xi}a = 0.5829a$$

$$L_l = \frac{\xi(7\phi+2) + (5\phi-3) + \frac{2}{\xi}(8-3\phi)}{31}a = 1.0200a$$

$$R_e = \frac{\phi\sqrt{\xi(\xi+\phi)+1}}{2}a = 2.0971a$$

$$\phi = \frac{1+\sqrt{5}}{2} \qquad \xi = \sqrt[3]{\frac{\phi + \sqrt{\phi - 5/27}}{2}} + \sqrt[3]{\frac{\phi - \sqrt{\phi - 5/27}}{2}}$$

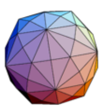
$$V = \frac{5\sqrt{\xi[\xi^2(11405\phi+287) + \xi(14528\phi+8265) + (2363\phi+131416)]}}{62}a^3 = 37.59a^3$$

$$S = 55.28a^2$$

$$[3]\text{: } R_v = \frac{\sqrt{3\left(\xi\phi + \phi + 1 + \frac{1}{\xi}\right)}}{2}a = 2.1172a$$

$$[5]\text{: } R_v = \frac{\sqrt{\xi^2[(1067\phi+1009) + \xi(2259\phi+1168) + (941\phi+1097)]}}{62}a = 2.2000a$$

$$R_i = \frac{\xi\sqrt{209[\xi^2(104\phi-7) + \xi(153\phi+52) + (195-\phi)]}}{418}a = 2.0399a$$



Disdyakis Triacontahedron

Vertices: 62 (30[4] + 20[6] + 12[10])

Faces: 120 (acute triangles)

Edges: 180 = $60L_s + 60L_{lm} + 60L_l$

Dual solid: Truncated Icosidodecahedron

$$V = \frac{180(5+4\sqrt{5})}{11}a^3 = 228.18a^3 \qquad S = \frac{180}{11}\sqrt{179 - 24\sqrt{5}}a^2 = 183.20a^2$$

$$L_s = \frac{\sqrt{15(85-31\sqrt{5})}}{11}a = 1.3943a$$

$$L_m = \frac{3\sqrt{15(65+19\sqrt{5})}}{55}a = 2.1902a$$

$$L_l = \frac{2\sqrt{15(5-\sqrt{5})}}{5}a = 2.5755a$$

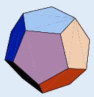
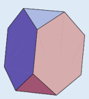
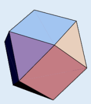
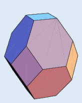
$$[4]\text{: } R_v = \frac{3(5+4\sqrt{5})}{11}a = 3.8030a$$

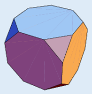
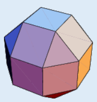
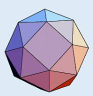
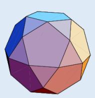
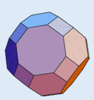
$$[6]\text{: } R_v = \sqrt{15}a = 3.8730a$$

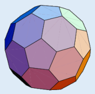
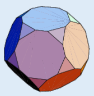
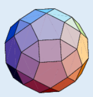
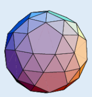
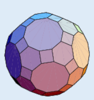
$$[10]\text{: } R_v = \frac{3\sqrt{5(5+2\sqrt{5})}}{5}a = 4.1291a$$

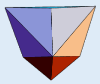
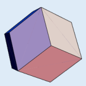
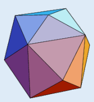
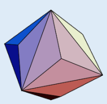
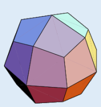
$$R_e = \frac{\sqrt{6(5+2\sqrt{5})}}{2}a = 3.7694a \qquad R_i = \frac{\sqrt{10845(39+16\sqrt{5})}}{241}a = 3.7366a$$

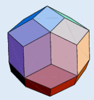
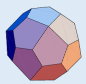
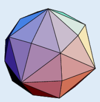
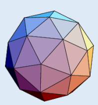
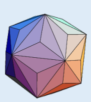
Table S1. Overview and summary of parameters from equations for polyhedra in Section 1 above.[S1]

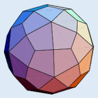
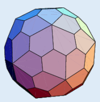
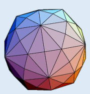
⇣ **Platonic and Archimedean Solids** ⇣											
Polyhedron	V	S	R_c	V_{Rc}/V	S_{Rc}/S	R_m	V_{Rm}/V	S_{Rm}/S	R_i	V_{Ri}/V	S_{Ri}/S
 Icosahedron	2.182	8.66	0.9511	1.65	1.31	0.8090	1.02	0.95	0.7558	0.83	0.83
 Dodecahedron	7.663	20.65	1.4010	1.50	1.19	1.3090	1.23	1.04	1.1140	0.76	0.76
 Truncated Tetrahedron	2.711	12.12	1.1726	2.49	1.43	1.0606	1.84	1.17	[3] 1.0206	1.64	1.08
									[6] 0.6123	0.35	0.39
 Cuboctahedron	2.357	9.464	1.0000	1.78	1.33	0.8660	1.15	1.00	[3] 0.8165	0.97	0.89
									[4] 0.7071	0.63	0.66
 Truncated Octahedron	11.31	26.78	1.5811	1.46	1.17	1.5000	1.25	1.06	[4] 1.4142	1.05	0.94
									[6] 1.2247	0.68	0.70

 Truncated Cube	13.56	32.43	1.7789	1.74	1.23	1.7071	1.54	1.13	[3] 1.6825	1.47	1.10
									[8] 1.2071	0.54	0.56
 Rhombicubocta-hedron	8.714	21.46	1.3990	1.32	1.15	1.3066	1.07	1.00	[3] 1.2743	0.99	0.95
									[4] 1.2071	0.85	0.85
 Snub Cube	7.890	18.86	1.3437	1.29	1.20	1.2472	1.03	1.04	[3] 1.2134	0.95	0.98
									[4] 1.1426	0.79	0.87
 Icosidodecahedron	13.84	29.31	1.6180	1.28	1.12	1.5388	1.10	1.02	[3] 1.5115	1.05	0.98
									[5] 1.3764	0.79	0.81
 Truncated Cuboctahedron	41.79	61.76	2.3176	1.25	1.09	2.2630	1.16	1.04	[4] 2.2071	1.08	0.99
									[6] 2.0908	0.92	0.89
									[8] 1.9142	0.70	0.75

 Truncated Icosahedron	55.29	72.61	2.4780	1.15	1.06	2.4271	1.08	1.02	[5] 2.3274	0.96	0.94
									[6] 2.2672	0.88	0.89
 Truncated Dodecahedron	85.04	100.99	2.9695	1.29	1.10	2.9271	1.24	1.07	[3] 2.9128	1.22	1.06
									[10] 2.4990	0.77	0.78
 Rhombicosido-decahedron	41.62	59.31	2.2330	1.12	1.06	2.1763	1.04	1.00	[3] 2.1571	1.01	0.99
									[4] 2.1180	0.96	0.95
									[5] 2.0653	0.89	0.90
 Snub Dodecahedron	37.62	55.289	2.1558	1.12	1.06	2.0971	1.03	1.00	[3] 2.0771	1.00	0.98
									[5] 1.9809	0.87	0.89
 Truncated Icosidodecahedron	206.8	175.03	3.8024	1.11	1.04	3.7694	1.08	1.02	[4] 3.7361	1.06	1.00
									[6] 3.6685	1.00	0.97

				⇣ Catalan Solids ⇣							
 Triakis Tetrahedron	5.7276	17.91	[3] 1.1023	0.98	0.85	1.0607	0.87	0.79	0.9594	0.65	0.65
			[6] 1.8371	4.53	2.37						
 Rhombic Dodecahedron	2.3865	9.546	[3] 0.9186	1.36	1.11	0.9428	1.47	1.17	0.7500	0.74	0.74
			[4] 1.0607	2.09	1.48						
 Tetrakis Hexahedron	14.32	30.91	[4] 1.5910	1.18	1.03	1.5000	0.99	0.91	1.4230	0.84	0.82
			[6] 1.8371	1.81	1.37						
 Triakis Octahedron	23.31	42.69	[3] 1.7321	0.93	0.88	1.7072	0.89	0.86	1.6383	0.79	0.79
			[8] 2.2414	2.02	1.48						
 Deltoidal Icositetrahedron	8.7507	21.51	[3] 1.3397	1.15	1.05	1.3066	1.07	1.00	1.2203	0.87	0.87
			[4] 1.4142	1.35	1.17						

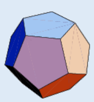
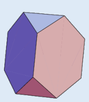
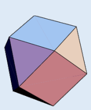
 Rhombic Triacontahedron	14.80	30.34	[3] 1.5667	1.09	1.02	1.5388	1.03	0.98	1.4635	0.89	0.89
			[5] 1.7204	1.44	1.23						
 Pentagonal Icositetrahedron	7.4474	19.30	[3] 1.2820	1.19	1.07	1.2472	1.09	1.01	1.1577	0.87	0.87
			[4] 1.3614	1.42	1.21						
 Disdyakis Dodecahedron	46.66	67.42	[4] 2.3204	1.12	1.00	2.2630	1.04	0.95	2.2097	0.97	0.91
			[6] 2.4495	1.32	1.12						
			[8] 2.6754	1.72	1.33						
 Pentakis Dodecahedron	59.88	75.56	[5] 2.5309	1.13	1.07	2.4271	1.00	0.98	2.3771	0.94	0.94
			[6] 2.5981	1.23	1.12						
 Triakis Icosahedron	111.15	115.57	[3] 2.9414	0.96	0.94	2.9271	0.95	0.93	2.8853	0.91	0.91
			[10] 3.4410	1.54	1.29						

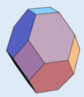
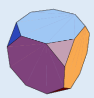
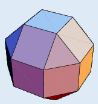
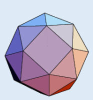
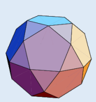
 Deltoidal Hexecontahedron	42.26	59.77	[3] 2.1957	1.05	1.01	2.1763	1.02	1.00	2.1210	0.95	0.95
			[4] 2.2361	1.11	1.05						
			[5] 2.2940	1.20	1.11						
 Pentagonal Hexecontahedron	37.59	55.28	[3] 2.1172	1.06	1.02	2.0971	1.03	1.00	2.0399	0.95	0.95
			[5] 2.2000	1.19	1.10						
 Disdyakis Triacontahedron	7.20	[4] 1.89	7.14	7.07	1548.4	91.1	92.0	89.6	87.2	1.010	0.983
		[6] 1.86	7.01	6.95	1466.0	86.2	92.0	84.8	82.6	1.066	0.983
		[10] 1.74	6.57	6.52	1209.8	71.2	92.0	70.0	68.2	1.292	0.983

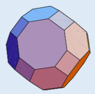
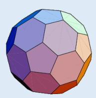
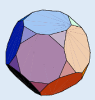
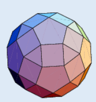
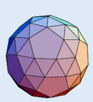
Section S2 – Data for polyhedra

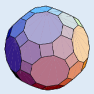
Table S2A. Calculated numbers of gold atoms in various polyhedra assuming a radius of the circumscribed sphere of **10.08 Å** (*i.e.* a Au_{147} cluster with regular icosahedral shape) and ratios between the number of gold atoms in the volume described by the circumscribed sphere (midscribed sphere or edge-scribed sphere) and the number of gold atoms obtained for each polyhedron assuming a sphere with vertex radius N_c / N_v, N_m / N_v or N_i / N_v. N_c is the number of gold atoms contained within the circumscribed sphere, N_v the number of gold atoms calculated from the volume of the polyhedron, and N_{ve} is the number of gold atoms calculated from the volume of the sphere with vertex radius in Catalan solids ($N_{ve} = V_{Rv} / V_{Au}$), N_m is the number of gold atoms calculated from the volume of the sphere with midscribed radius ($N_m = V_{Rm} / V_{Au}$), and N_e is the number of gold atoms calculated from the volume of the sphere with edge-scribed radius ($N_{es} = V_{Re} / V_{Au}$). R_i = radius of the inscribed sphere, R_m = radius of the midscribed sphere, R_e = radius of the edge-scribed sphere, R_v = vertex radius (numbers in square brackets denote faces of polygons, *e.g.*, [3] for triangle, [5] for pentagon, *etc.*), V is the calculated volume of the polyhedron, L is the edge length of the polyhedron, a is the edge length of dual solid in Catalan solids, and N_i is the number of gold atoms in the inscribed sphere. Models taken from: Polyèdres, http://wwwmathcurvecom/polyedres/polyedresshtml

⇣ Platonic and Archimedean Solids ⇣

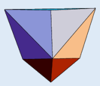
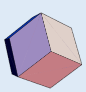
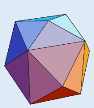
	Polyhedron	R_c / Å	L / Å	R_m / Å	R_i / Å	V / Å^3	N_v	N_c	N_m	N_i	N_c / N_v	N_m / N_v	N_i / N_v
	Icosahedron	10.08	10.60	8.57	8.01	2597.51	152.8	252.4	155.3	126.6	1.65	1.02	0.83
	Dodecahedron	10.08	7.19	9.42	8.01	2852.25	167.8	252.4	205.7	126.6	1.50	1.23	0.75
	Truncated Tetrahedron	10.08	8.60	9.12	[3] 8.77	1722.11	101.3	252.4	186.7	166.4	2.49	1.84	1.64
					[6] 5.26					35.9			0.35
	Cuboctahedron	10.08	10.08	8.73	[3] 8.23	2414.02	142.0	252.4	163.9	137.4	1.78	1.15	0.97

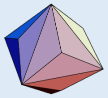
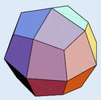
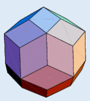
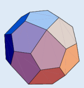
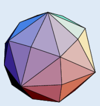
				[4] 7.13					89.2			0.63
 Truncated Octahedron	10.08	6.38	9.56	[4] 9.02	2930.67	172.4	252.4	215.5	180.6	1.46	1.25	1.05
				[6] 7.81					117.3			0.68
 Truncated Cube	10.08	5.67	9.67	[3] 9.53	2467.10	145.1	252.4	223.0	213.5	1.74	1.54	1.47
				[8] 6.84					78.8			0.54
 Rhombicuboctahedron	10.08	7.21	9.41	[3] 9.18	3259.46	191.7	252.4	205.6	190.7	1.32	1.07	0.99
				[4] 8.70					162.1			0.85
 Snub Cube	10.08	7.50	9.36	[3] 9.10	3330.61	195.9	252.4	201.8	185.8	1.29	1.03	0.95
				[4] 8.57					155.2			0.79
 Icosidodecahedron	10.08	6.23	9.59	[3] 9.42	3346.43	196.8	252.4	217.1	205.7	1.28	1.10	1.05
				[5] 8.57					155.4			0.79

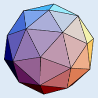
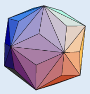
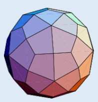
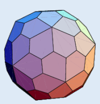
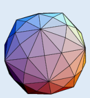
 Truncated Cuboctahedron	10.08	4.35	9.84	[4] 9.60	3438.26	202.3	252.4	234.9	218.0	1.25	1.16	1.08
				[6] 9.09					185.3			0.92
				[8] 8.33					142.2			0.70
 Truncated Icosahedron	10.08	4.07	9.87	[5] 9.47	3721.55	218.9	252.4	237.1	209.1	1.15	1.08	0.96
				[6] 9.22					193.3			0.88
 Truncated Dodecahedron	10.08	3.39	9.94	[3] 9.89	3326.25	195.7	252.4	241.7	238.2	1.29	1.24	1.22
				[10] 8.48					150.4			0.77
 Rhombicosido-decahedron	10.08	4.51	9.82	[3] 9.74	3828.40	225.2	252.4	233.6	227.5	1.12	1.04	1.01
				[4] 9.56					215.3			0.96
				[5] 9.32					199.7			0.89
 Snub Dodecahedron	10.08	4.68	9.81	[3] 9.71	3845.70	226.2	252.4	232.3	225.7	1.12	1.03	1.00

					[5] 9.26					195.8			0.87
	Truncated Icosidodecahedron	10.08	2.65	9.99	[4] 9.90	3852.64	226.6	252.4	245.8	239.4	1.11	1.08	1.06
					[6] 9.73					226.6			1.00

⇣ Catalan Solids ⇣

	Polyhedron	R_v / Å	a / Å	R_e / Å	R_i / Å	V / Å^3	N_v	N_{ve}	N_e	N_i	N_{ve} / N_v	N_{es} / N_v	N_i / N_v
	Triakis Tetrahedron	10.80	[3] 9.14	9.70	8.77	4379.81	257.6	252.4	224.9	166.4	0.980	0.873	0.646
			[6] 5.49	5.82	5.26	946.14	55.7	252.4	48.6	35.9	4.534	0.873	0.646
	Rhombic Dodecahedron	10.80	[3] 10.97	10.35	8.23	3153.29	185.5	252.4	272.8	137.3	1.361	1.471	0.740
			[4] 9.50	8.96	7.13	2048.17	120.5	252.4	177.2	89.2	2.095	1.471	0.740
	Tetrakis Hexahedron	10.80	[4] 6.34	9.50	9.02	3641.78	214.2	252.4	211.5	180.6	1.178	0.987	0.843
			[6] 5.49	8.23	7.81	2365.52	139.1	252.4	137.4	117.3	1.814	0.987	0.843

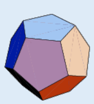
 Triakis Octahedron	10.80	[3] 5.82	9.94	9.53	4594.15	270.2	252.4	241.6	213.5	0.934	0.894	0.790
		[8] 4.50	7.68	7.37	2120.09	124.7	252.4	111.5	98.5	2.024	0.894	0.790
 Deltoidal Icositetrahedron	10.80	[3] 7.52	9.83	9.18	3727.36	219.3	252.4	234.1	190.7	1.151	1.068	0.870
		[4] 7.13	9.31	8.70	3168.78	186.4	252.4	199.0	162.1	1.354	1.068	0.870
 Rhombic Triacontahedron	10.80	[3] 6.43	9.90	9.42	3941.72	231.9	252.4	239.1	205.7	1.088	1.031	0.887
		[5] 5.86	9.02	8.57	2976.84	175.1	252.4	180.6	155.3	1.441	1.031	0.887
 Pentagonal Icositetrahedron	10.80	[3] 7.86	9.81	9.10	3620.11	212.9	252.4	232.4	185.8	1.185	1.091	0.873
		[4] 7.40	9.23	8.57	3022.94	177.8	252.4	194.0	155.2	1.419	1.091	0.873
 Disdyakis Dodecahedron	10.80	[4] 4.34	9.83	9.60	3825.37	225.0	252.4	234.1	217.9	1.121	1.040	0.969
		[6] 4.12	9.31	9.09	3251.84	191.3	252.4	199.0	185.3	1.319	1.040	0.969
		[8] 3.77	8.53	8.33	2495.72	146.8	252.4	152.7	142.2	1.719	1.040	0.969

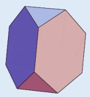
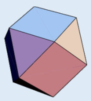
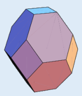
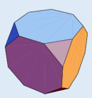
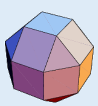
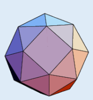
 Pentakis Dodecahedron	10.80	[5] 3.98	9.67	9.47	3783.02	222.5	252.4	222.6	209.1	1.134	1.000	0.940
		[6] 3.88	9.42	9.22	3497.00	205.7	252.4	205.7	193.3	1.227	1.000	0.940
 Triakis Icosahedron	10.80	[3] 3.43	10.03	9.89	4473.31	263.1	252.4	248.7	238.2	0.959	0.945	0.905
		[10] 2.93	8.57	8.45	2794.07	164.4	252.4	155.3	148.8	1.535	0.945	0.905
 Deltoidal Hexecontahedron	10.80	[3] 4.59	9.99	9.74	4088.76	240.5	252.4	245.7	227.5	1.049	1.022	0.946
		[4] 4.51	9.81	9.56	3871.13	227.7	252.4	232.7	215.4	1.108	1.022	0.946
		[5] 4.39	9.56	9.32	3585.34	210.9	252.4	215.5	199.5	1.197	1.022	0.946
 Pentagonal Hexecontahedron	10.80	[3] 4.76	9.98	9.71	4056.66	238.6	252.4	245.2	225.7	1.058	1.028	0.946
		[5] 4.58	9.61	9.35	3615.65	212.7	252.4	218.6	201.2	1.187	1.028	0.946
 Disdyakis Triacontahedron	10.80	[4] 2.65	9.99	9.90	4248.94	249.9	252.4	245.7	239.4	1.010	0.983	0.958
		[6] 2.60	9.81	9.73	4022.69	236.6	252.4	232.6	226.6	1.066	0.983	0.958

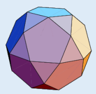
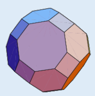
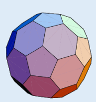
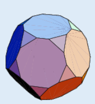
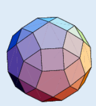
		[10] 2.44	9.20	9.12	3319.66	195.3	252.4	192.0	187.0	1.292	0.983	0.958

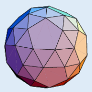
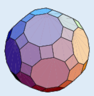
Table S2B. Calculated numbers of gold atoms in various polyhedra assuming a radius of the circumscribed sphere of **7.20 Å** (*i.e.* a Au_{55} cluster with regular icosahedral shape) and ratios between the number of gold atoms in the volume described by the circumscribed sphere (midscribed sphere or edge-scribed sphere) and the number of gold atoms obtained for each polyhedron assuming a sphere with vertex radius N_c / N_v, N_m / N_v or N_i / N_v. N_c is the number of gold atoms contained within the circumscribed sphere, N_v the number of gold atoms calculated from the volume of the polyhedron, and N_{ve} is the number of gold atoms calculated from the volume of the sphere with vertex radius in Catalan solids ($N_{ve} = V_{Rv} / V_{Au}$), N_m is the number of gold atoms calculated from the volume of the sphere with midscribed radius ($N_m = V_{Rm} / V_{Au}$), and N_e is the number of gold atoms calculated from the volume of the sphere with edge-scribed radius ($N_e = V_{Re} / V_{Au}$). R_i = radius of the inscribed sphere, R_m = radius of the midscribed sphere, R_e = radius of the edge-scribed sphere, R_v = vertex radius (numbers in square brackets denote faces of polygons, *e.g.*, [3] for triangle, [5] for pentagon, etc.), V is the calculated volume of the polyhedron, L is the edge length of the polyhedron, a is the edge length of dual solid in Catalan solids, and N_i is the number of gold atoms in the inscribed sphere. [S1]

⇣ Platonic and Archimedean Solids ⇣

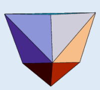
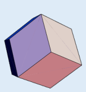
Polyhedron	R_c / Å	L / Å	R_m / Å	R_i / Å	V / Å^3	N_v	N_c	N_m	N_i	N_c / N_v	N_m / N_v	N_i / N_v
 Icosahedron	7.20	7.57	6.12	5.72	946.62	55.7	92.0	56.6	46.2	1.652	1.016	0.829
 Dodecahedron	7.20	5.14	6.73	5.72	1039.45	61.1	92.0	75.0	46.1	1.504	1.226	0.755

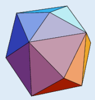
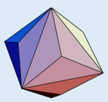
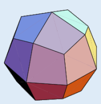
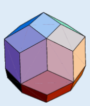
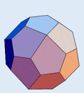
 Truncated Tetrahedron	7.20	6.14	6.51	[3] 6.27	627.59	36.9	92.0	68.1	60.6	2.491	1.843	1.643
				[6] 3.76					13.1			0.355
 Cuboctahedron	7.20	7.20	6.24	[3] 5.88	879.75	51.7	92.0	59.7	50.1	1.777	1.154	0.967
				[4] 5.09					32.5			0.628
 Truncated Octahedron	7.20	4.55	6.83	[4] 6.44	1068.03	62.8	92.0	78.5	65.8	1.464	1.250	1.048
				[6] 5.58					42.7			0.680
 Truncated Cube	7.20	4.05	6.91	[3] 6.81	899.09	52.9	92.0	81.3	77.8	1.739	1.537	1.471
				[8] 4.89					28.7			0.543
 Rhombicuboctahedron	7.20	5.15	6.72	[3] 6.56	1187.85	69.9	92.0	74.9	69.5	1.316	1.072	0.995
				[4] 6.21					59.1			0.845
 Snub Cube	7.20	5.36	6.68	[3] 6.50	1213.78	71.4	92.0	73.5	67.7	1.288	1.030	0.949

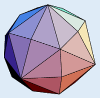
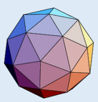
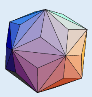
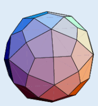
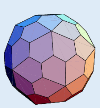
				[4] 6.12					56.5			0.792
 Icosidodecahedron	7.20	4.45	6.85	[3] 6.73	1219.55	71.7	92.0	79.1	75.0	1.282	1.103	1.045
				[5] 6.12					56.6			0.789
 Truncated Cuboctahedron	7.20	4.35	7.03	[4] 6.86	1253.01	73.7	92.0	85.6	79.4	1.248	1.162	1.078
				[6] 6.50					67.5			0.916
				[8] 5.95					51.8			0.703
 Truncated Icosahedron	7.20	4.07	7.05	[5] 6.76	1356.25	79.8	92.0	86.4	76.2	1.153	1.083	0.955
				[6] 6.59					70.4			0.883
 Truncated Dodecahedron	7.20	3.39	7.10	[3] 7.06	1212.19	71.3	92.0	88.1	86.8	1.290	1.235	1.217
				[10] 6.06					54.8			0.769
 Rhombicosido-decahedron	7.20	4.51	7.02	[3] 6.96	1395.19	82.1	92.0	85.1	82.9	1.121	1.037	1.010

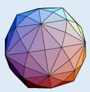
					[4] 6.83					78.5			0.956
					[5] 6.66					72.8			0.887
	Snub Dodecahedron	7.20	4.68	7.00	[3] 6.94	1401.49	82.4	92.0	84.7	82.3	1.116	1.027	0.998
					[5] 6.62					71.4			0.865
	Truncated Icosidodecahedron	7.20	2.65	7.14	[4] 7.07	1404.02	82.6	92.0	89.6	87.2	1.114	1.085	1.056
					[6] 6.95					82.6			1.000

⇣ Catalan Solids ⇣

	Polyhedron	R_v / Å	a / Å	R_e / Å	R_i / Å	V / Å^3	N_v	N_{ve}	N_e	N_i	N_{ve} / N_v	N_{es} / N_v	N_i / N_v
	Triakis Tetrahedron	7.20	[3] 6.53	6.93	6.27	1596.1	93.9	92.0	81.9	60.6	0.980	0.873	0.646
			[6] 3.92	4.16	3.76	344.8	20.3	92.0	17.7	13.1	4.534	0.873	0.646
	Rhombic Dodecahedron	7.20	[3] 7.84	7.39	5.88	1149.2	67.6	92.0	99.4	50.1	1.361	1.471	0.740

		[4] 6.79	6.40	5.09	746.4	43.9	92.0	64.6	32.5	2.095	1.471	0.740
 Tetrakis Hexahedron	7.20	[4] 4.53	6.79	6.44	1327.2	78.1	92.0	77.1	65.8	1.178	0.987	0.843
		[6] 3.92	5.88	5.58	862.1	50.7	92.0	50.1	42.7	1.814	0.987	0.843
 Triakis Octahedron	7.20	[3] 4.16	7.10	6.81	1674.3	98.5	92.0	88.1	77.8	0.934	0.894	0.790
		[8] 3.21	5.48	5.26	772.6	45.4	92.0	40.6	35.9	2.024	0.894	0.790
 Deltoidal Icositetrahedron	7.20	[3] 5.37	7.02	6.56	1358.4	79.9	92.0	85.3	69.5	1.151	1.068	0.870
		[4] 5.09	6.65	6.21	1154.8	67.9	92.0	72.5	59.1	1.354	1.068	0.870
 Rhombic Triacontahedron	7.20	[3] 4.60	7.07	6.73	1436.5	84.5	92.0	87.1	75.0	1.088	1.031	0.887
		[5] 4.19	6.44	6.12	1084.9	63.8	92.0	65.8	56.6	1.441	1.031	0.887
 Pentagonal Icositetrahedron	7.20	[3] 5.62	7.00	6.50	1319.3	77.6	92.0	84.7	67.7	1.185	1.091	0.873
		[4] 5.29	6.60	6.12	1101.7	64.8	92.0	70.7	56.6	1.419	1.091	0.873

 Disdyakis Dodecahedron	7.20	[4] 3.10	7.02	6.86	1394.1	82.0	92.0	85.3	79.4	1.121	1.040	0.969
		[6] 2.94	6.65	6.50	1185.1	69.7	92.0	72.5	67.5	1.319	1.040	0.969
		[8] 2.69	6.09	5.95	909.5	53.5	92.0	55.7	51.8	1.719	1.040	0.969
 Pentakis Dodecahedron	7.20	[5] 2.84	6.90	6.76	1378.7	81.1	92.0	81.1	76.2	1.134	1.000	0.940
		[6] 2.77	6.73	6.59	1274.4	75.0	92.0	75.0	70.4	1.227	1.000	0.940
 Triakis Icosahedron	7.20	[3] 2.45	7.16	7.06	1630.2	95.9	92.0	90.6	86.8	0.959	0.945	0.905
		[10] 2.09	6.12	6.04	1018.2	59.9	92.0	56.6	54.2	1.535	0.945	0.905
 Deltoidal Hexecontahedron	7.20	[3] 3.28	7.14	6.96	1490.1	87.7	92.0	89.6	82.9	1.049	1.022	0.946
		[4] 3.22	7.01	6.83	1410.8	83.0	92.0	84.8	78.5	1.108	1.022	0.946
		[5] 3.14	6.83	6.66	1306.6	76.9	92.0	78.5	72.7	1.197	1.022	0.946
 Pentagonal Hexecontahedron	7.20	[3] 3.40	7.13	6.94	1478.4	87.0	92.0	89.4	82.3	1.058	1.028	0.946

		[5] 3.27	6.86	6.68	1317.7	77.5	92.0	79.7	73.3	1.187	1.028	0.946
 Disdyakis Triacontahedron	7.20	[4] 1.89	7.14	7.07	1548.4	91.1	92.0	89.6	87.2	1.010	0.983	0.958
		[6] 1.86	7.01	6.95	1466.0	86.2	92.0	84.8	82.6	1.066	0.983	0.958
		[10] 1.74	6.57	6.52	1209.8	71.2	92.0	70.0	68.2	1.292	0.983	0.958

Section S3 – Data for Archimedean Icosahedra

Table S3. List of Archimedean icosahedron clusters (for abbreviations see Table 4 in the main text).

Polyhedron	***G***	**Cluster**	**Surface**	D_c / nm	D_m / nm	D_i / nm	N_v	N_c	N_m	N_i	N_v / N	N_c / N	N_m / N	N_i / N
Icosahedron 13	1	13	12	0.864	0.735	0.687	12.0	19.9	12.2	10.0	0.93	1.53	0.94	0.77
Dodecahedron 33	2	33	20	1.203	1.124	0.956	35.7	53.7	43.8	26.9	1.08	1.63	1.33	0.82
Icosidodecahedron 43	2	43	30	1.268	1.206	[3] 1.184	49.0	62.8	54.0	51.2	1.14	1.46	1.26	1.19
						[4] 1.079				38.6				0.90
Icosahedron 55	2	55	42	1.440	1.225	1.144	55.7	92.0	56.6	46.2	1.01	1.67	1.03	0.84
Dodecahedron 75	3	75	32	1.680	1.570	1.335	97.1	146.1	119.1	73.3	1.30	1.95	1.59	0.98
Rhombicosido-	3	115	60	1.717	1.674	[3] 1.659	139.2	156.0	144.4	140.6	1.21	1.36	1.26	1.22

decahedron 115														
						[4] 1.629				133.1				1.16
						[5] 1.588				123.4				1.07
Truncated Icosahedron 135	3	135	80	1.758	1.722	[5] 1.651	145.1	167.3	157.2	138.6	1.07	1.24	1.16	1.03
						[6] 1.608				128.1				0.95
Icosidodecahedron 145	3	145	90	1.867	1.776	[3] 1.744	156.4	200.5	172.5	163.5	1.08	1.38	1.19	1.13
						[5] 1.588				123.4				0.85
Icosahedron 147	3	147	92	2.016	1.715	1.602	152.8	252.4	155.3	126.6	1.04	1.72	1.06	0.86
Dodecahedron 165	3	165	110	2.175	2.031	1.728	210.6	316.7	258.2	158.9	1.28	1.92	1.56	0.96
Truncated Dodecahedron 195	4	195	140	2.119	2.089	[3] 2.078	227.2	293.0	280.6	276.5	1.17	1.50	1.44	1.42
						[10] 1.783				174.6				0.90
Rhombicosido-decahedron 207	4	207	72	2.119	2.065	[3] 2.047	261.5	293.0	271.2	264.1	1.26	1.42	1.31	1.28
						[4] 2.010				250.0				1.21
						[5] 1.960				231.8				1.12
Icosidodecahedron 237	4	237	102	2.268	2.157	[3] 2.119	280.3	359.4	309.2	293.0	1.18	1.52	1.30	1.24
						[5] 1.930				221.3				0.93
Sub-Rhombicosi-	4	267	120	2.182	2.126	[3] 2.107	285.4	319.8	296.0	288.3	1.07	1.20	1.11	1.08

dodecahedron 267														
						[4] 2.069				272.9				1.02
						[5] 2.018				253.0				0.95
Icosahedron 309	4	309	162	2.592	2.205	2.060	324.7	536.4	330.1	269.2	1.05	1.74	1.07	1.01
Sub-Truncated Icosahedron 327	4	327	180	2.453	2.403	[5] 2.304	394.4	454.7	427.2	376.7	1.21	1.39	1.31	1.15
						[6] 2.244				348.2				1.06
Truncated Dodecahedron 357	5	357	120	2.627	2.589	[3] 2.577	432.8	558.2	534.7	526.9	1.21	1.56	1.50	1.48
						[10] 2.211				332.7				0.93
Sub-Rhombico-sidodecahedron 387	5	387	120	2.493	2.430	[3] 2.409	426.0	477.4	441.9	430.3	1.10	1.23	1.14	1.11
						[4] 2.365				407.3				1.05
						[5] 2.306				377.7				0.98
Truncated Dodecahedron 447	5	417	180	2.738	2.699	[3] 2.686	490.0	632.0	605.4	596.5	1.18	1.52	1.45	1.43
						[10] 2.304				376.7				0.90
Sub-Rhombico-sidodecahedron 429	5	429	132	2.667	2.600	[3] 2.577	521.6	584.5	541.1	526.9	1.22	1.36	1.26	1.23
						[4] 2.530				498.7				1.16

						[5] 2.467				462.4				1.08
Truncated Icosido-decahedron 437	5	437	140	2.671	2.647	[4] 2.624	526.9	586.7	571.5	556.5	1.21	1.34	1.31	1.27
						[6] 2.577				526.9				1.21
						[12] 2.417				434.8				0.99
Dodecahedron 467	5	437	210	3.086	2.883	2.452	602.0	905.4	738.0	454.3	1.38	2.07	1.69	1.04
Sub-Truncated Icosahedron 489	5	489	192	2.738	2.681	[5] 2.571	548.2	632.0	593.8	523.6	1.12	1.29	1.21	1.07
						[6] 2.505				484.0				0.99
Sub-Icosahedron 509	5	509	200	3.028	2.576	2.407	517.9	855.4	526.4	429.3	1.02	1.68	1.03	0.84
Icosahedron 561	5	561	252	3.168	2.695	2.517	592.9	979.3	602.7	491.4	1.06	1.75	1.07	0.88
Sub-Truncated Icosahedron 599	5	599	290	2.918	2.858	[5] 2.740	663.6	765.0	718.9	633.9	1.11	1.28	1.20	1.06
						[6] 2.670				585.9				0.98
Snub Dodecahedron (enantiomer) 629	6	629	200	3.149	3.064	[3] 3.034	862.5	962.2	885.7	860.6	1.37	1.53	1.41	1.37
						[5] 2.894				746.5				1.19

Truncated Dodecahedron 669	6	669	240	3.093	3.049	[3] 3.034	706.9	911.7	873.2	860.5	1.06	1.36	1.31	1.29
						[10] 2.603				543.4				0.81
Truncated Icosido-decahedron 689	6	689	260	3.064	3.037	[4] 3.010	795.3	885.6	862.7	840.1	1.15	1.29	1.25	1.22
						[6] 2.956				795.3				1.15
						[12] 2.772				656.3				0.95
Rhombicosido-decahedron 789	6	789	360	3.114	3.035	[3] 3.008	829.8	929.9	860.9	838.3	1.05	1.18	1.09	1.06
						[4] 2.953				793.5				1.01
						[5] 2.880				735.7				0.93
Sub-Truncated Icosidodecahedron 839	6	839	402	3.182	3.155	[4] 3.127	891.5	992.8	967.1	941.7	1.06	1.18	1.15	1.12
						[6] 3.070				891.5				1.06
						[12] 2.880				735.7				0.88
Truncated Icosahedron 851	6	851	302	3.228	3.161	[5] 3.031	898.4	1034	973.1	858.1	1.06	1.22	1.14	1.01
						[6] 2.953				793.2				0.93
Icosahedron 923	6	923	362	3.744	3.185	2.975	978.7	1616	994.8	811.1	1.06	1.75	1.08	0.88
Dodecahedron 1019	6	1019	570	4.349	4.063	3.456	1685	2534	2066	1271	1.65	2.49	2.03	1.38

Section S4 – Data for Archimedean Cubes

Table S4. List of Archimedean cubes (for abbreviations see Table 5 in the main text).

Polyhedron	G	Cluster	Surface	D_c / nm	D_m / nm	D_i / nm	N_v	N_c	N_m	N_i	N_v / N	N_c / N	N_m / N	N_i / N
Cuboctahedron 13	1	13	12	0.983	0.852	[3] 0.803	16.5	29.3	19.0	15.9	1.27	2.25	1.46	1.23
						[4] 0.695				10.4				0.80
Truncated Octahedron 38	2	38	32	1.233	1.169	[4] 1.103	39.4	57.7	49.3	41.3	1.04	1.52	1.30	1.09
						[6] 0.955				26.8				0.71
Rhombicuboctahedron 43	2	43	30	1.278	1.193	[3] 1.164	48.8	64.3	52.4	48.6	1.14	1.49	1.22	1.13
						[4] 1.103				41.3				0.96
Cuboctahedron 55	2	55	42	1.559	1.350	[3] 1.273	65.7	116.8	75.8	63.6	1.19	2.12	1.38	1.16
						[4] 1.103				41.3				0.75
Truncated Cube 62	2	62	48	1.625	1.559	[3] 1.537	76.0	132.1	116.8	111.8	1.23	2.13	1.88	1.80
						[8] 1.103				41.3				0.67
Sub-Truncated Octahedron 79	3	79	60	1.688	1.601	[4] 1.510	101.2	148.2	126.5	106.0	1.28	1.88	1.60	1.34
						[6] 1.308				68.9				0.87
Sub-Rhombicubocta-hedron 92	3	92	54	1.750	1.634	[3] 1.594	125.4	165.0	134.5	124.7	1.36	1.79	1.46	1.36
						[4] 1.510				106.0				1.15

Snub Cube 111	3	111	56	1.776	1.648	[3] 1.603	133.9	172.4	137.9	127.0	1.21	1.55	1.24	1.14
						[4] 1.510				106.0				0.96
Sub-Truncated Octahedron 116	3	116	78	1.688	1.601	[4] 1.510	101.2	148.2	126.5	106.0	0.87	1.28	1.09	0.91
						[6] 1.308				68.9				0.59
Truncated Cuboctahedron 135	3	135	80	1.828	1.764	[4] 1.741	150.8	188.2	169.0	162.5	1.12	1.39	1.25	1.20
						[6] 1.649				138.2				1.02
						[8] 1.510				106.0				0.79
Sub-Rhombicubocta-hedron 140	3	140	78	1.750	1.634	[3] 1.594	125.4	165.0	134.5	124.7	0.90	1.18	0.96	0.89
						[4] 1.510				106.0				0.76
Cuboctahedron 147	3	147	92	2.135	1.849	[3] 1.743	168.7	299.9	194.8	163.2	1.15	2.04	1.32	1.11
						[4] 1.510				106.0				0.72
Truncated Cube 164	3	164	102	2.225	2.135	[3] 2.105	195.1	339.3	299.9	287.1	1.19	2.07	1.83	1.75
						[8] 1.510				106.0				0.65
Sub-Truncated Cube 171	3	171	108	2.225	2.135	[3] 2.105	195.1	339.3	299.9	287.1	1.14	1.98	1.75	1.68
						[8] 1.510				106.0				0.62
Sub-Truncated Octahedron 140	4	140	96	2.143	2.033	[4] 1.917	207.2	303.3	259.0	217.0	1.48	2.17	1.85	1.55
						[6] 1.660				141.0				1.01

Sub-Rhombicubocta-hedron 165	4	165	86	2.222	2.075	[3] 2.024	256.7	337.9	275.3	255.3	1.56	2.05	1.67	1.55
						[4] 1.917				217.0				1.32
Truncated Octahedron 201	4	201	122	2.143	2.033	[4] 1.917	207.2	303.3	259.0	217.0	1.03	1.51	1.29	1.08
						[6] 1.660				141.0				0.70
Sub-Cuboctahedron 260	4	260	144	2.711	2.348	[3] 2.214	345.4	613.9	398.7	334.2	1.33	2.36	1.53	1.29
						[4] 1.917				217.0				0.83
Sub-Truncated Cuboctahedron 236	4	236	120	2.321	2.239	[4] 2.211	308.7	385.2	345.9	332.7	1.31	1.63	1.47	1.41
						[6] 2.094				282.8				1.20
						[8] 1.917				217.0				0.92
Sub-Rhombicubocta-hedron 249	4	249	114	2.222	2.075	[3] 2.024	256.7	337.9	275.3	255.3	1.03	1.36	1.11	1.03
						[4] 1.917				217.0				0.87
Sub-Snub Cube 249	4	249	114	2.255	2.093	[3] 2.036	274.0	353.0	282.3	259.9	1.10	1.42	1.13	1.04
						[4] 1.917				217.0				0.87
Sub-Snub Cube 268	4	268	128	2.255	2.093	[3] 2.036	274.0	353.0	282.3	259.9	1.02	1.32	1.05	0.97
						[4] 1.917				217.0				0.81
Sub-Truncated Cuboctahedron 297	4	297	162	2.321	2.239	[4] 2.211	308.7	385.2	345.9	332.7	1.04	1.30	1.16	1.12

						[6] 2.094				282.8				0.95
						[8] 1.917				217.0				0.73
Cuboctahedron 309	4	309	162	2.711	2.348	[3] 2.214	345.4	613.9	398.7	334.2	1.12	1.99	1.29	1.08
						[4] 1.917				217.0				0.70
Sub-Truncated Cuboctahedron 316	4	316	152	2.321	2.239	[4] 2.211	308.7	385.2	345.9	332.7	0.98	1.22	1.09	1.05
						[6] 2.094				282.8				0.90
						[8] 1.917				217.0				0.69
Sub-Rhombicubocta-hedron 321	4	321	150	2.222	2.075	[3] 2.024	256.7	337.9	275.3	255.3	0.80	1.05	0.86	0.80
						[4] 1.917				217.0				0.68
Cuboctahedron 340	4	340	176	2.711	2.348	[3] 2.214	345.4	613.9	398.7	334.2	1.02	1.81	1.17	0.98
						[4] 1.917				217.0				0.64
Truncated Cube 357	4	357	186	2.825	2.711	[3] 2.672	399.5	694.6	613.9	587.7	1.12	1.95	1.72	1.65
						[8] 1.917				217.0				0.61
Sub-Cube 364	4	364	192	3.321	2.711	1.917	414.5	1127.8	613.9	217.0	1.14	3.10	1.69	0.60
Sub-Octahedron 225	5	225	140	2.324	1.644	1.342	123.1	386.8	136.8	74.4	0.55	1.72	0.61	0.33
Sub-Rhombicubocta-hedron 266	5	266	126	2.694	2.516	[3] 2.454	457.5	602.2	490.5	455.1	1.72	2.26	1.84	1.71
						[4] 2.324				386.8				1.45
Sub-Truncated Octahedron 314	5	314	174	2.599	2.465	[4] 2.324	369.3	540.5	461.6	386.8	1.18	1.72	1.47	1.23

						[6] 2.013				251.2				0.80
Sub-Rhombicubocta-hedron 369	5	369	168	2.694	2.516	[3] 2.454	457.5	602.2	490.5	455.1	1.24	1.63	1.33	1.23
						[4] 2.324				386.8				1.05
Rhombicuboctahedron 394	5	394	158	2.694	2.516	[3] 2.454	457.5	602.2	490.5	455.1	1.16	1.53	1.25	1.15
						[4] 2.324				386.8				0.98
Sub-Snub Cube 394	5	394	158	2.733	2.537	[3] 2.468	488.4	629.1	503.0	463.2	1.24	1.60	1.28	1.18
						[4] 2.324				386.8				0.98
Sub-Truncated Octahedron 405	5	405	204	2.599	2.465	[4] 2.324	369.3	540.5	461.6	386.8	0.91	1.33	1.14	0.96
						[6] 2.013				251.2				0.62
Snub Cube 429	5	429	132	2.733	2.537	[3] 2.468	488.4	629.1	503.0	463.2	1.14	1.47	1.17	1.08
						[4] 2.324				386.8				0.90
Sub-Truncated Cuboctahedron 466	5	466	230	2.814	2.715	[4] 2.680	550.2	686.5	616.5	592.9	1.18	1.47	1.32	1.27
						[6] 2.539				504.0				1.08
						[8] 2.324				386.8				0.83
Sub-Cuboctahedron 490	5	490	230	3.287	2.847	[3] 2.684	615.6	1094.1	710.5	595.5	1.26	2.23	1.45	1.22
						[4] 2.324				386.8				0.79
Sub-Truncated	5	501	204	2.814	2.715	[4] 2.680	550.2	686.5	616.5	592.9	1.10	1.37	1.23	1.18

Cuboctahedron 501														
						[6] 2.539				504.0				1.01
						[8] 2.324				386.8				0.77
Sub-Rhombicubocta-hedron 514	5	514	198	2.694	2.516	[3] 2.454	457.5	602.2	490.5	455.1	0.89	1.17	0.95	0.89
						[4] 2.324				386.8				0.75
Sub-Cuboctahedron 549	5	549	240	3.287	2.847	[3] 2.684	615.6	1094.1	710.5	595.5	1.12	1.99	1.29	1.08
						[4] 2.324				386.8				0.70
Cuboctahedron 561	5	561	252	3.287	2.847	[3] 2.684	615.6	1094.1	710.5	595.5	1.10	1.95	1.27	1.06
						[4] 2.324				386.8				0.69
Sub-Truncated Cuboctahedron 586	5	586	246	2.814	2.715	[4] 2.680	550.2	686.5	616.5	592.9	0.94	1.18	1.06	1.02
						[6] 2.539				504.0				0.86
						[8] 2.324				386.8				0.66
Sub-Truncated Cuboctahedron 605	5	605	248	2.814	2.715	[4] 2.680	550.2	686.5	616.5	592.9	0.91	1.13	1.02	0.98
						[6] 2.539				504.0				0.83
						[8] 2.324				386.8				0.64
Sub-Cuboctahedron 610	5	610	270	3.287	2.847	[3] 2.684	615.6	1094.1	710.5	595.5	1.01	1.79	1.16	0.98
						[4] 2.324				386.8				0.63

Sub-Truncated Cube 641	5	641	284	3.425	3.287	[3] 3.240	711.9	1238.0	1094.0	1047.4	1.11	1.93	1.71	1.63
						[8] 2.324				386.8				0.60
Sub-Truncated Cube 658	5	658	294	3.425	3.287	[3] 3.240	711.9	1238.0	1094.0	1047.4	1.08	1.88	1.66	1.59
						[8] 2.324				386.8				0.59
Sub-Octahedron 338	6	338	192	2.732	1.932	1.577	199.9	627.9	222.0	120.8	0.59	1.86	0.66	0.36
Sub-Octahedron 399	6	394	174	2.732	1.932	1.577	199.9	627.9	222.0	120.8	0.51	1.59	0.56	0.31
Sub-Truncated Octahedron 459	6	459	234	3.054	2.898	[4] 2.732	599.4	877.5	749.3	627.9	1.31	1.91	1.63	1.37
						[6] 2.366				407.8				0.89
Rhombicuboctahedron 579	6	579	210	3.166	2.957	[3] 2.884	742.7	977.5	796.3	738.7	1.28	1.69	1.38	1.28
						[4] 2.732				627.9				1.08
Truncated Octahedron 586	6	586	272	3.054	2.898	[4] 2.732	599.4	877.5	749.3	627.9	1.02	1.50	1.28	1.07
						[6] 2.366				407.8				0.70
Sub-Truncated Cuboctahedron 675	6	675	270	3.308	3.191	[4] 3.150	893.1	1114.4	1000.8	962.5	1.32	1.65	1.48	1.43
						[6] 2.984				818.2				1.21
						[8] 2.732				627.9				0.93
Sub-Rhombicubocta-	6	730	264	3.166	2.957	[3] 2.884	742.7	977.5	796.3	738.7	1.02	1.34	1.09	1.01

hedron 730														
						[4] 2.732				627.9				0.86
Rhombicubocta-hedron 755	6	755	254	3.166	2.957	[3] 2.884	742.7	977.5	796.3	738.7	0.98	1.29	1.05	0.98
						[4] 2.732				627.9				0.83
Snub Cube 755	6	755	254	3.213	2.982	[3] 2.901	792.8	1021.2	816.6	752.0	1.05	1.35	1.08	1.00
						[4] 2.732				627.9				0.83
Sub-Truncated Octahedron 802	6	802	312	3.054	2.898	[4] 2.732	599.4	877.5	749.3	627.9	0.75	1.09	0.93	0.78
						[6] 2.366				407.8				0.51
Truncated Cuboctahedron 863	6	863	314	3.308	3.191	[4] 3.150	893.1	1114.4	1000.8	962.5	1.03	1.29	1.16	1.12
						[6] 2.984				818.2				0.95
						[8] 2.732				627.9				0.73
Sub-Truncated Octahedron 898	6	898	312	3.054	2.898	[4] 2.732	599.4	877.5	749.3	627.9	0.67	0.98	0.84	0.70
						[6] 2.366				407.8				0.46
Sub-Cuboctahedron 911	6	911	350	3.863	3.346	[3] 3.154	999.4	1776.0	1153.5	966.8	1.10	1.95	1.27	1.06
						[4] 2.732				627.9				0.69
Cuboctahedron 923	6	923	362	3.863	3.346	[3] 3.154	999.4	1776.0	1153.5	966.8	1.08	1.92	1.25	1.05
						[4] 2.732				627.9				0.68

Sub-Truncated Cuboctahedron 970	6	970	360	3.308	3.191	[4] 3.150	893.1	1114.4	1000.8	962.5	0.92	1.15	1.03	0.99
						[6] 2.984				818.2				0.84
						[8] 2.732				627.9				0.65
Sub-Truncated Cube 1043	6	1043	402	4.026	3.863	[3] 3.808	1155.7	2009.7	1776.0	1700.3	1.11	1.93	1.70	1.63
						[8] 2.732				627.9				0.60
Truncated Cube 1074	6	1074	416	4.026	3.863	[3] 3.808	1155.7	2009.7	1776.0	1700.3	1.08	1.87	1.65	1.58
						[8] 2.732				627.9				0.58
Sub-Truncated Cube 1091	6	1091	426	4.026	3.863	[3] 3.808	1155.7	2009.7	1776.0	1700.3	1.06	1.84	1.63	1.56
						[8] 2.732				627.9				0.58

Section S5 – Example calculations

The expected structures (closest or best match) of several gold nanoparticles synthesized by our group[S2-S5] are summarized in Table S5 (high resolution TEM images are available free of charge in the electronic supporting information in most cases). The models used are listed and those highlighted in red font were considered the closest match to the gold nanoparticles experimentally observed in the TEM images. The gold nanoparticles Au1, Au2, Au4, Au5, Au10, and Au11 (No. 7, 8, 10, 11, 16, 17) had TEM images with sufficiently high resolution (see images in the original papers and their supporting information), making the choice for the most appropriate model easy (as outlined in the main text, a sufficiently high quality of TEM images is important). The structures and compositions of the other gold nanoparticles were estimated from their size distribution histograms.

The estimated core structures of the gold nanoparticles reported by Negishi *et al.*[S6] are shown in Table S6. Their structures have previously been estimated *via* DFT calculations. Our models and tables help analyze them and select the best match for the core structure.

Table S5. Lists of gold nanoparticles and their model structures.

No.	Ref.	Au-NP	D / nm	Model	D_c / nm	D_m / nm	D_i / nm	h / nm	w / nm
1	[S2]	Au-*R***1**	2.47 ± 0.18	Truncated Icosidodecahedron 437	2.671	2.647	[4] 2.624 [6] 2.577 [12] 2.417		
				Sub-Truncated Cuboctahedron 466	2.814	2.715	[4] 2.680 [6] 2.539 [8] 2.324		
				Sub-Truncated Icosahedron 489	2.738	2.681	[5] 2.571 [6] 2.505		
2	[S2]	Au-*R***2**	2.13 ± 0.18	Sub-Rhombicosidodecahedron 267	2.182	2.126	[3] 2.107 [4] 2.069 [5] 2.018		
				Sub-Truncated Cuboctahedron 297	2.321	2.239	[4] 2.211 [6] 2.094		

							[8] 1.917		
				Icosahedron 309	2.592	2.205	2.060		
3	[S2]	Au-*R***3**	1.24 ± 0.28	Icosahedron 55	1.440	1.225	1.144		
				Ino's Decahedron 55				1.44	1.32
				Cuboctahedron 55	1.559	1.350	[3] 1.273 [4] 1.103		
4		Au-*S***1**	1.73 ± 0.20	Icosidodecahedron 145	1.867	1.776	[3] 1.744 [5] 1.588		
				Icosahedron 147	2.016	1.715	1.602		
				Cuboctahedron 147	2.135	1.849	[3] 1.743 [4] 1.510		
				Dodecahedron 165	2.175	2.031	1.728		
5	[S2]	Au-*S***2**	1.08 ± 0.24	Marks' Decahedron 29				1.15	1.09
6	[S2]	Au-*S***3**	1.09 ± 0.23	Dodecahedron 33	1.203	1.124	0.956		
				Truncated Octahedron 38	1.233	1.169	[4] 1.103 [6] 0.955		
				Ino's Decahedron 39				1.15	1.32
7	[S3]	Au1	1.65 ± 0.39	Ino's Decahedron 116				1.73	1.83
				Marks' Decahedron 146				1.73	2.12
				Truncated Icosahedron 135	1.758	1.722	[5] 1.651 [6] 1.608		
				Sub-Truncated Octahedron 116	1.688	1.601	[4] 1.510 [6] 1.308		
				Cuboctahedron 147	2.135	1.849	[3] 1.743 [4] 1.510		
8	[S3]	Au2	1.54 ± 0.38	Ino's Decahedron 71				1.73	1.32

				Marks' Decahedron 75				1.44	1.61
				Dodecahedron 75	1.680	1.570	1.335		
				Sub-Truncated Octahedron 116	1.688	1.601	[4] 1.510 [6] 1.308		
9	[S3, S4]	Au3	3.50 ± 0.81	—[a]					
10		Au4	1.20 ± 0.23	Marks' Decahedron 29				1.15	1.09
				Ino's Decahedron 39				1.15	1.32
				Icosidodecahedron 43	1.268	1.206	[3] 1.184 [4] 1.079		
				Truncated Octahedron 38	1.233	1.169	[4] 1.103 [6] 0.955		
11	[S3]	Au5	1.75 ± 0.40	Marks' Decahedron 146				1.73	2.12
				Ino's Decahedron 147				2.02	1.83
				Icosahedron 147	2.016	1.715	1.602		
				Cuboctahedron 147	2.135	1.849	[3] 1.743 [4] 1.510		
				Truncated Octahedron 201	2.143	2.033	[4] 1.917 [6] 1.660		
12	[S3]	Au6	—[a]						
13	[S3]	Au7	1.58 ± 0.44	Marks' Decahedron 101				1.44	1.83
				Rhombicosidodecahedron 115	1.717	1.674	[3] 1.659 [4] 1.629 [5] 1.588		
				Sub-Truncated Octahedron 116	1.688	1.601	[4] 1.510 [6] 1.308		
14	[S3]	Au8	1.93 ± 0.47	Marks' Decahedron 238				2.30	2.12

				Icosidodecahedron 237	2.268	2.157	[3] 2.119 [5] 1.930		
				Truncated Octahedron 201	2.143	2.033	[4] 1.917 [6] 1.660		
				Sub-Rhombicuboctahedron 249	2.222	2.075	[3] 2.024 [4] 1.917		
15	[S3]	Au9	1.31 ± 0.29	Ino's Decahedron 71				1.73	1.32
				Icosahedron 55	1.440	1.225	1.144		
				Cuboctahedron 55	1.559	1.350	[3] 1.273 [4] 1.103		
16	[S3]	Au10	1.57 ± 0.43	Marks' Decahedron 101				1.73	1.61
				Rhombicosidodecahedron 115	1.717	1.674	[3] 1.659 [4] 1.629 [5] 1.588		
				Sub-Truncated Octahedron 116	1.688	1.601	[4] 1.510 [6] 1.308		
17	[S3]	Au11	1.61 ± 0.42	Marks' Decahedron 101				1.73	1.61
				Truncated Icosahedron 135	1.758	1.722	[5] 1.651 [6] 1.608		
				Icosahedron 147	2.016	1.715	1.602		
				Sub-Truncated Octahedron 116	1.688	1.601	[4] 1.510 [6] 1.308		
				Cuboctahedron 147	2.135	1.849	[3] 1.743 [4]		

No.	Ref.	Au-NP	*D* / nm	Model	D_c / nm	D_m / nm	D_i / nm
							1.510
18	[S5]	AuNP1	4.09	Cuboctahedron 1415	4.439	3.844	[3] 3.625 [4] 3.139
				Sub-Truncated Cuboctahedron 1416	3.801	3.667	[4] 3.619 [6] 3.429 [8] 3.139

[a] Could not be isolated in pure form (and analyzed here) due to amphiphilicity of the resulting mixed-monolayer-protected Au NPs.

Table S6. Lists of gold nanoparticles and their core structures.

No.	Ref.	Au-NP	*D* / nm	Model	D_c / nm	D_m / nm	D_i / nm
19	[S6]	$Au_{\sim 226}(SC_{12})_{\sim 76}$	2.0 ± 0.5	Truncated Octahedron 201	2.143	2.033	[4] 1.917 [6] 1.660
				Sub-Truncated Cuboctahedron 236	2.321	2.239	[4] 2.211 [6] 2.094 [8] 1.917
20	[S6]	$Au_{\sim 253}(SC_{12})_{\sim 90}$	2.1 ± 0.4	Sub-Truncated Cuboctahedron 236	2.321	2.239	[4] 2.211 [6] 2.094 [8] 1.917
				Sub-Rhombicuboctahedron 249	2.222	2.075	[3] 2.024 [4] 1.917
21	[S6]	$Au_{329}(SC_{12})_{84}$	2.2 ± 0.4	Sub-Truncated Cuboctahedron 297	2.321	2.239	[4] 2.211 [6] 2.094 [8] 1.917
				Cuboctahedron 309	2.711	2.348	[3] 2.214 [4]

				Sub-Truncated Cuboctahedron 316	2.321	2.239	1.917 [4] 2.211 [6] 2.094 [8] 1.917
22	[S6]	$Au_{\sim356}(SC_{12})_{\sim112}$	2.2 ± 0.3	Cuboctahedron 340	2.711	2.348	[3] 2.214 [4] 1.917
				Sub-Truncated Octahedron 314	2.599	2.465	[4] 2.324 [6] 2.013
23	[S6]	$Au_{\sim520}(SC_{12})_{\sim130}$	2.4 ± 0.2	Sub-Truncated Cuboctahedron 466	2.814	2.715	[4] 2.680 [6] 2.539 [8] 2.324
				Sub-Cuboctahedron 490	3.287	2.847	[3] 2.684 [4] 2.324
				Sub-Truncated Cuboctahedron 501	2.814	2.715	[4] 2.680 [6] 2.539 [8] 2.324

Section S6 – *xyz* Coordinates

The xzy-coordinates for all gold nanoclusters are provided as separate electronic supplementary materials. These xyz-coordinate files are provided in standard format that can be analyzed just like crystal structures using CIF format.

References

[S1] Models and equations from: Wolfram MathWorld, http://mathworld.wolfram.com/ and Visual Polyhedra, http://dmccooey.com/polyhedra/index.html

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[S4] Qi, H.; Hegmann, T. Formation of Periodic Stripe Patterns in Nematic Liquid Crystals Doped with Functionalized Gold Nanoparticles. *J. Mater. Chem.* **16**, 4197-4205 (2006).
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