# Polyhedra in (Inorganic) Chemistry

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## Electronic Supplementary Information

**Table S1**. Complete list of the Johnson polyhedra, ordered according to the number of vertices (V), giving the number of edges (E) and faces (F) in each case.

**Table S2.** Nested polyhedra that appear as successive shells in prototypical solid state structures. The shells are ordered according to increasing distance to the center.

**Table S3.** Nested polyhedra of icosahedral symmetry in the molecular structure of $[Pd_{145}(CO)_x(PEt_3)_{30}]$.

**Figure S1.** Polyhedra generated from a dodecahedron through augmentation and truncation operations.

**Figure S2.** Polyhedra generated from a cube through augmentation and truncation operations.

**Figure S3.** Diamond shells 2 and 6 around centroid of adamantanoid unit, forming an octahedron and a truncated octahedron.

**Figure S4.** Generation of an approximate icosahedron of bridging selenide ions in an $Ag_8$ cube in the molecular structure of $Ag_8Cl_2[Se_2P(OEt)_2]_6$.

**Table S1**. Complete list of the Johnson polyhedra, ordered according to the number of vertices (V), giving the number of edges (E) and faces (F) in each case.

| Name (number) | V | E | F |
|---|---|---|---|
| square pyramid (J1) | 5 | 8 | $4_3 + 1_4 = 5$ |
| triangular dipyramid (J12) | 5 | 9 | $6_3 = 6$ |
| pentagonal pyramid (J2) | 6 | 10 | $5_3 + 1_5 = 6$ |
| elongated triangular pyramid (J7) | 7 | 12 | $4_3 + 3_4 = 7$ |
| pentagonal dipyramid (J13) | 7 | 15 | $10_3 = 10$ |
| augmented triangular prism (J49) | 7 | 13 | $6_3 + 3_4 = 8$ |
| elongated triangular dipyramid (J14) | 8 | 15 | $6_3 + 3_4 = 9$ |
| gyrobifastigium (J26) | 8 | 14 | $4_3 + 4_4 = 8$ |
| biaugmented triangular prism (J50) | 8 | 17 | $10_3 + 1_4 = 11$ |
| snub disphenoid (J84) | 8 | 18 | $12_3 = 12$ |
| triangular cupola (J3) | 9 | 15 | $4_3 + 3_4 + 1_6 = 8$ |
| elongated square pyramid (J8) | 9 | 16 | $4_3 + 5_5 = 9$ |
| gyroelongated square pyramid (J10) | 9 | 20 | $12_3 + 1_4 = 13$ |
| triaugmented triangular prism (J51) | 9 | 21 | $14_3 = 14$ |
| tridiminished icosahedron (J63) | 9 | 15 | $5_3 + 3_5 = 8$ |
| elongated square dipyramid (J15) | 10 | 20 | $8_3 + 4_4 = 12$ |
| gyroelongated square dipyramid (J17) | 10 | 24 | $16_3 = 16$ |
| metabidiminished icosahedron (J62) | 10 | 20 | $10_3 + 2_5 = 12$ |
| augmented tridiminished icosahedron (J64) | 10 | 18 | $7_3 + 3_5 = 10$ |
| sphenocorona (J86) | 10 | 22 | $12_3 + 2_4 = 14$ |
| elongated pentagonal pyramid (J9) | 11 | 20 | $5_3 + 5_4 + 1_5 = 11$ |
| gyroelongated pentagonal pyramid (J11) | 11 | 25 | $15_3 + 1_5 = 16$ |
| augmented pentagonal prism (J52) | 11 | 19 | $4_3 + 4_4 + 2_5 = 10$ |
| augmented sphenocorona (J87) | 11 | 26 | $16_3 + 1_4 = 17$ |
| square cupola (J4) | 12 | 20 | $4_3 + 5_4 + 1_8 = 10$ |
| elongated pentagonal dipyramid (J16) | 12 | 25 | $10_3 + 5_4 = 15$ |
| triangular orthobicupola (J27) | 12 | 24 | $8_3 + 6_4 = 14$ |
| biaugmented pentagonal prism (J53) | 12 | 23 | $8_3 + 3_4 + 2_5 = 13$ |
| sphenomegacorona (J88) | 12 | 28 | $16_3 + 2_4 = 18$ |
| augmented hexagonal prism (J54) | 13 | 22 | $4_3 + 5_4 + 2_6 = 11$ |
| parabiaugmented hexagonal prism (J55) | 14 | 26 | $8_3 + 4_4 + 2_6 = 14$ |
| metabiaugmented hexagonal prism (J56) | 14 | 26 | $8_3 + 4_4 + 2_6 = 14$ |
| hebesphenomegacorona (J89) | 14 | 22 | $18_3 + 2_4 = 21$ |
| bilunabirotunda (J91) | 14 | 26 | $8_3 + 2_4 + 4_5 = 14$ |

| | | | |
|---|---|---|---|
| pentagonal cupola (J5) | 15 | 25 | $5_3 + 5_4 + 1_5 + 1_{10} = 12$ |
| elongated triangular cupola (J18) | 15 | 27 | $4_3 + 9_4 + 1_6 = 14$ |
| gyroelongated triangular cupola (J22) | 15 | 33 | $16_3 + 3_4 + 1_6 = 20$ |
| triaugmented hexagonal prism (J57) | 15 | 30 | $12_3 + 3_4 + 2_6 = 17$ |
| augmented truncated tetrahedron (J65) | 15 | 27 | $8_3 + 3_4 + 3_6 = 14$ |
| square orthobicupola (J28) | 16 | 32 | $8_3 + 10_4 = 18$ |
| square gyrobicupola (J29) | 16 | 32 | $8_3 + 10_4 = 18$ |
| snub square antiprism (J85) | 16 | 40 | $24_3 + 2_4 = 26$ |
| disphenocingulum (J90) | 16 | 38 | $20_3 + 4_4 = 24$ |
| elongated triangular orthobicupola (J35) | 18 | 36 | $8_3 + 12_4 = 20$ |
| elongated triangular gyrobicupola (J36) | 18 | 36 | $8_3 + 12_4 = 20$ |
| gyroelongated triangular bicupola (J44) | 18 | 42 | $20_3 + 6_4 = 26$ |
| triangular hebesphenorotunda (J92) | 18 | 36 | $13_3 + 3_4 + 3_5 + 1_6 = 20$ |
| pentagonal rotunda (J6) | 20 | 35 | $10_3 + 6_5 + 1_{10} = 17$ |
| elongated square cupola (J19) | 20 | 36 | $4_3 + 13_4 + 1_8 = 18$ |
| gyroelongated square cupola (J23) | 20 | 44 | $20_3 + 5_4 + 1_8 = 26$ |
| pentagonal orthobicupola (J30) | 20 | 40 | $10_3 + 10_4 + 2_5 = 22$ |
| pentagonal gyrobicupola (J31) | 20 | 40 | $10_3 + 10_4 + 2_5 = 22$ |
| parabiaugmented dodecahedron (J59) | 22 | 40 | $10_3 + 10_5 = 20$ |
| metabiaugmented dodecahedron (J60) | 22 | 42 | $10_3 + 10_5 = 20$ |
| triaugmented dodecahedron (J61) | 23 | 45 | $15_3 + 9_5 = 24$ |
| elongated square gyrobicupola (J37) | 24 | 48 | $8_3 + 18_4 = 26$ |
| gyroelongated square bicupola (J45) | 24 | 56 | $24_3 + 10_4 = 34$ |
| elongated pentagonal cupola (J20) | 25 | 45 | $5_3 + 15_4 + 1_5 + 1_{10} = 22$ |
| gyroelongated pentagonal cupola (J24) | 25 | 55 | $25_3 + 5_4 + 1_5 + 1_{10} = 32$ |
| pentagonal orthocupolarontunda (J32) | 25 | 50 | $15_3 + 5_4 + 7_5 = 27$ |
| pentagonal gyrocupolarotunda (J33) | 25 | 50 | $15_3 + 5_4 + 7_5 = 27$ |
| augmented truncated cube (J66) | 28 | 48 | $12_3 + 5_4 + 5_8 = 22$ |
| elongated pentagonal rotunda (J21) | 30 | 55 | $10_3 + 10_4 + 6_5 + 1_{10} = 27$ |
| gyroelongated pentagonal rotunda (J25) | 30 | 65 | $30_3 + 6_5 + 1_{10} = 37$ |
| elongated pentagonal orthobicupola (J38) | 30 | 60 | $10_3 + 20_4 + 2_5 = 32$ |
| elongated pentagonal gyrobicupola (J39) | 30 | 60 | $10_3 + 20_4 + 2_5 = 32$ |
| gyroelongated pentagonal bicupola (J46) | 30 | 70 | $30_3 + 10_4 + 2_5 = 42$ |
| biaugmented truncated cube (J67) | 30 | 60 | $16_3 + 10_4 + 4_8 = 32$ |
| elongated pentagonal orthocupolarotunda (J40) | 35 | 60 | $15_3 + 15_4 + 7_5 = 37$ |
| elongated pentagonal gyrocupolarotunda (J41) | 35 | 60 | $15_3 + 15_4 + 7_5 = 37$ |
| gyroelongated pentagonal cupolarotunda (J47) | 35 | 80 | $35_3 + 5_4 + 7_5 = 47$ |
| augmented dodecahedron (J58) | 35 | 21 | $5_3 + 11_5 = 16$ |

| | | | |
|---|---|---|---|
| elongated pentagonal orthobirotunda (J42) | 40 | 80 | $20_3 + 10_4 + 12_5 = 42$ |
| elongated pentagonal gyrobirotunda (J43) | 40 | 80 | $20_3 + 10_4 + 12_5 = 42$ |
| gyroelongated pentagonal birotunda (J48) | 40 | 90 | $40_3 + 12_5 = 52$ |
| tridiminished rhombicosidodecahedron (J83) | 45 | 75 | $5_3 + 15_4 + 9_5 + 3_{10} = 32$ |
| parabidiminished rhombicosidodecahedron (J80) | 50 | 90 | $10_3 + 20_4 + 10_5 + 2_{10} = 42$ |
| metabidiminished rhombicosidodecahedron (J81) | 50 | 90 | $10_3 + 20_4 + 10_5 + 2_{10} = 42$ |
| gyrate bidiminished rhombicosidodecahedron (J82) | 50 | 90 | $10_3 + 20_4 + 10_5 + 2_{10} = 42$ |
| diminished rhombicosidodecahedron (J76) | 55 | 105 | $15_3 + 25_4 + 11_5 + 1_{10} = 52$ |
| paragyrate diminished rhombicosidodecahedron (J77) | 55 | 105 | $15_3 + 25_4 + 11_5 + 1_{10} = 52$ |
| metagyrate diminished rhombicosidodecahedron (J78) | 55 | 105 | $15_3 + 25_4 + 11_5 + 1_{10} = 52$ |
| bigyrate diminished rhombicosidodecahedron (J79) | 55 | 105 | $15_3 + 25_4 + 11_5 + 1_{10} = 52$ |
| pentagonal orthobirotunda (J34) | 60 | 30 | $20_3 + 12_5 = 32$ |
| parabiaugmented truncated dodecahedron (J69) | 60 | 120 | $30_3 + 10_4 + 2_5 + 10_{10} = 52$ |
| gyrate rhombicosidodecahedron (J72) | 60 | 120 | $20_3 + 30_4 + 12_5 = 62$ |
| parabigyrate rhombicosidodecahedron (J73) | 60 | 120 | $20_3 + 30_4 + 12_5 = 62$ |
| metabigyrate rhombicosidodecahedron (J74) | 60 | 120 | $20_3 + 30_4 + 12_5 = 62$ |
| trigyrate rhombicosidodecahedron (J75) | 60 | 120 | $20_3 + 30_4 + 12_5 = 62$ |
| augmented truncated dodecahedron (J68) | 65 | 105 | $25_3 + 5_4 + 1_5 + 11_{10} = 42$ |
| metabiaugmented truncated dodecahedron (J70) | 70 | 120 | $30_3 + 10_4 + 2_5 + 10_{10} = 52$ |
| triaugmented truncated dodecahedron (J71) | 75 | 135 | $35_3 + 15_4 + 3_5 + 9_{10} = 62$ |

[†] The subindex indicates the order of the polygonal faces. E.g., $6_4 + 8_6$ means six tetragonal and eight hexagonal faces.

**Table S2.** Nested polyhedra that appear as successive shells in prototypical solid state structures. The shells are ordered according to increasing distance to the center.

| Shell | | Polyhedron * | Dist. to center | Total atoms |
|---|---|---|---|---|
| **bcc** | | | | |
| 1 | $M_8$ | Cube | 1.50 | 9 |
| 2 | $M_6$ | Octahedron | 1.73 | 15 |
| 3 | $M_{12}$ | Cuboctahedron | 2.45 | 27 |
| 4 | $M_{24}$ | *Rhombicuboctahedron* | 2.87 | 51 |
| 5 | $M_8$ | Cube | 3.00 | 59 |
| 6 | $M_6$ | Octahedron | 3.46 | 65 |
| 7 | $M_{24}$ | *Truncated cube* | 3.77 | 89 |
| 8 | $M_{24}$ | Truncated octahedron | 3.87 | 113 |
| 9 | $M_{24}$ | *Rhombicuboctahedron* | 4.24 | 137 |
| 10 | | compound: | | |
| | $M_{24}$ | *Rhombicuboctahedron* | 4.50 | 169 |
| | $M_8$ | Cube | 4.50 | 145 |
| 11 | $M_{12}$ | Cuboctahedron | 4.89 | 181 |
| 12 | $M_{48}$ | *Truncated cuboctahedron* | 5.15 | 229 |
| 13 | | compound: | | |
| | $M_{24}$ | *Truncated cube* | 5.19 | 253 |
| | $M_6$ | Octahedron | 5.19 | 259 |
| 14 | $M_{24}$ | *Truncated octahedron* | 5.47 | 273 |
| 15 | $M_{24}$ | *Rhomicuboctahedron* | 5.67 | 297 |
| **fcc** (around atomic site) | | | | |
| 1 | $M_{12}$ | Cuboctahedron | 3.2 | 13 |
| 2 | $M_6$ | Octahedron | 3.66 | 19 |
| 3 | $M_{24}$ | Rhombicuboctahedron | 4.48 | 43 |
| 4 | $M_{12}$ | Cuboctahedron | 5.17 | 55 |
| 5 | $M_{24}$ | Truncated octahedron | 5.78 | 79 |
| 6 | $M_8$ | Cube | 6.44 | 87 |
| 7 | $M_{48}$ | Truncated cuboctahedron | 6.84 | 135 |
| 8 | $M_6$ | Octahedron | 7.31 | 141 |
| 9a | $M_{24}$ | Rhombicuboctahedron | 7.76 | 165 |
| 9b | $M_{12}$ | Cuboctahedron | 7.76 | 177 |
| 10 | $M_{24}$ | Truncated octahedron | | 201 |

**fcc** (around octahedral hole)

| | | | | |
|---|---|---|---|---|
| 1 | $M_6$ | Octahedron | 1.83 | 6 |
| 2 | $M_8$ | Cube | 3.17 | 14 |
| 3 | $M_{24}$ | Truncated octahedron | 4.09 | 38 |
| 4 | $M_{24}$ | *Truncated cube* | 5.48 | 62 |
| 5 | $M_6$ | Octahedron | 5.48 | 68 |
| 6 | $M_{24}$ | *Rhombicuboctahedron* | 6.06 | 92 |
| 7 | $M_{24}$ | Truncated octahedron | 6.59 | 116 |
| 8 | $M_6$ | | | |
| 9a | $M_{24}$ | | | |
| 9b | $M_{12}$ | | | |
| 10 | $M_{24}$ | | | |

**diamond** (non centered)

| | | | | |
|---|---|---|---|---|
| 1 | $C_4$ | Tetrahedron | 1.54 | 4 |
| 2 | $C_6$ | Octahedron | 1.78 | 10 |
| 3 | $C_{12}$ | Truncatred tetrahedron | 2.95 | 22 |
| 4 | $C_8$ | Cube | 3.08 | 30 |
| 5 | $C_{12}$ | Truncated tetrahedron | 3.88 | 42 |
| 6 | $C_{24}$ | Truncated octahedron | 3.98 | 68 |

**diamond** (centered)

| | | | | |
|---|---|---|---|---|
| 1 | $C_4$ | Tetrahedron | 1.54 | 5 |
| 2 | $C_{12}$ | Cuboctahedron | 2.52 | 17 |
| 3 | $C_{12}$ | Truncated tetrahedron | 2.95 | 29 |
| 4 | $C_6$ | Octahedron | 3.56 | 35 |
| 5 | $C_{12}$ | Distorted cuboctahedron | 3.88 | 47 |
| 6 | $C_{24}$ | Rhombicuboctahedron | 4.36 | 71 |

* In italics, non-Archimedean version of those polyhedra (see text)

| Shell | Composition | Polyhedron | Dist. to center |
|-------|-------------|------------|-----------------|
| 1 | $Pd_{12}$ | Icosahedron | 2.6 |
| 2 | $Pd_{30}$ | Icosidodecahedron | 4.5 |
| 3 | $Pd_{12}$ | Icosahedron | 5.4 |
| 4 | $Pd_{60}$ | Rhombicosidodecahedron | 6.6 |
| 5 | $Pd_{30}$ | Icosidodecahedron | 8.2 |
| 6 | $P_{30}$ | Icosidodecahedron | 10.5 |

**Table S3.** Nested polyhedra of icosahedral symmetry in the molecular structure of $[Pd_{145}(CO)_x(PEt_3)_{30}]$.

Truncated icosahedron

Icosahedron

$A_F$

$A_E$

$T_{2e}$

$T_{2i}$

$T_f$

Icosidodecahedron

$T_e$

$T_r$

Truncated icosidodecahedron

Rhombicosidodecahedron

Truncated dodecahedron
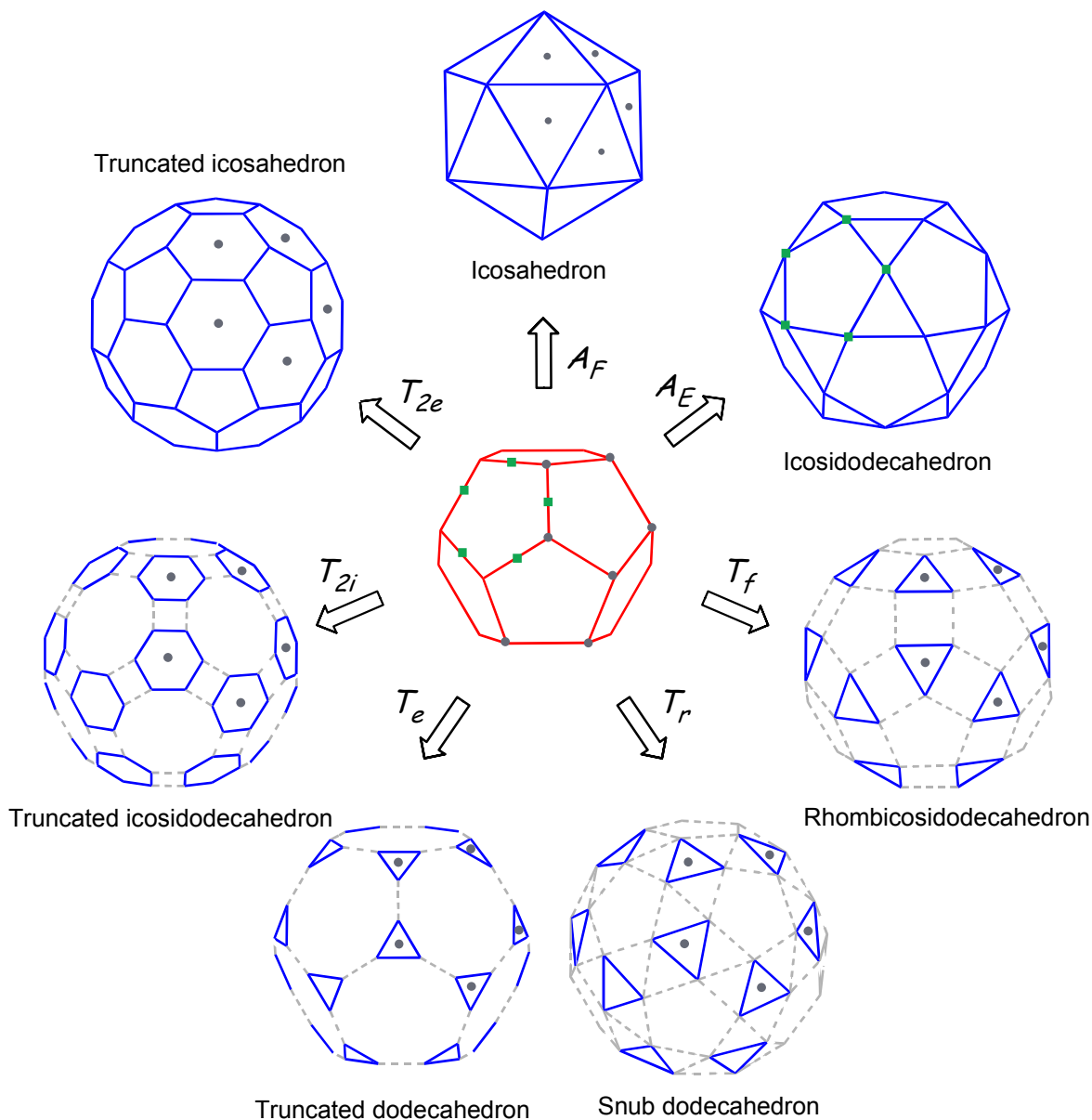
Snub dodecahedron

**Figure S1.** Polyhedra generated from a dodecahedron through the following operations: face augmentation ($A_F$), edge augmentation ($A_E$), face-directed truncation ($T_f$), rotated truncation ($T_r$), edge-directed truncation ($T_e$), and two double truncations with independent hexagons ($T_{2i}$) and with edge-sharing octagons ($T_{2e}$). The correspondence between some vertices of the octahedron and the faces of the generated polyhedra are noted with gray dots, that between edges of the octahedron and vertices of the cuboctahedron with green squares.
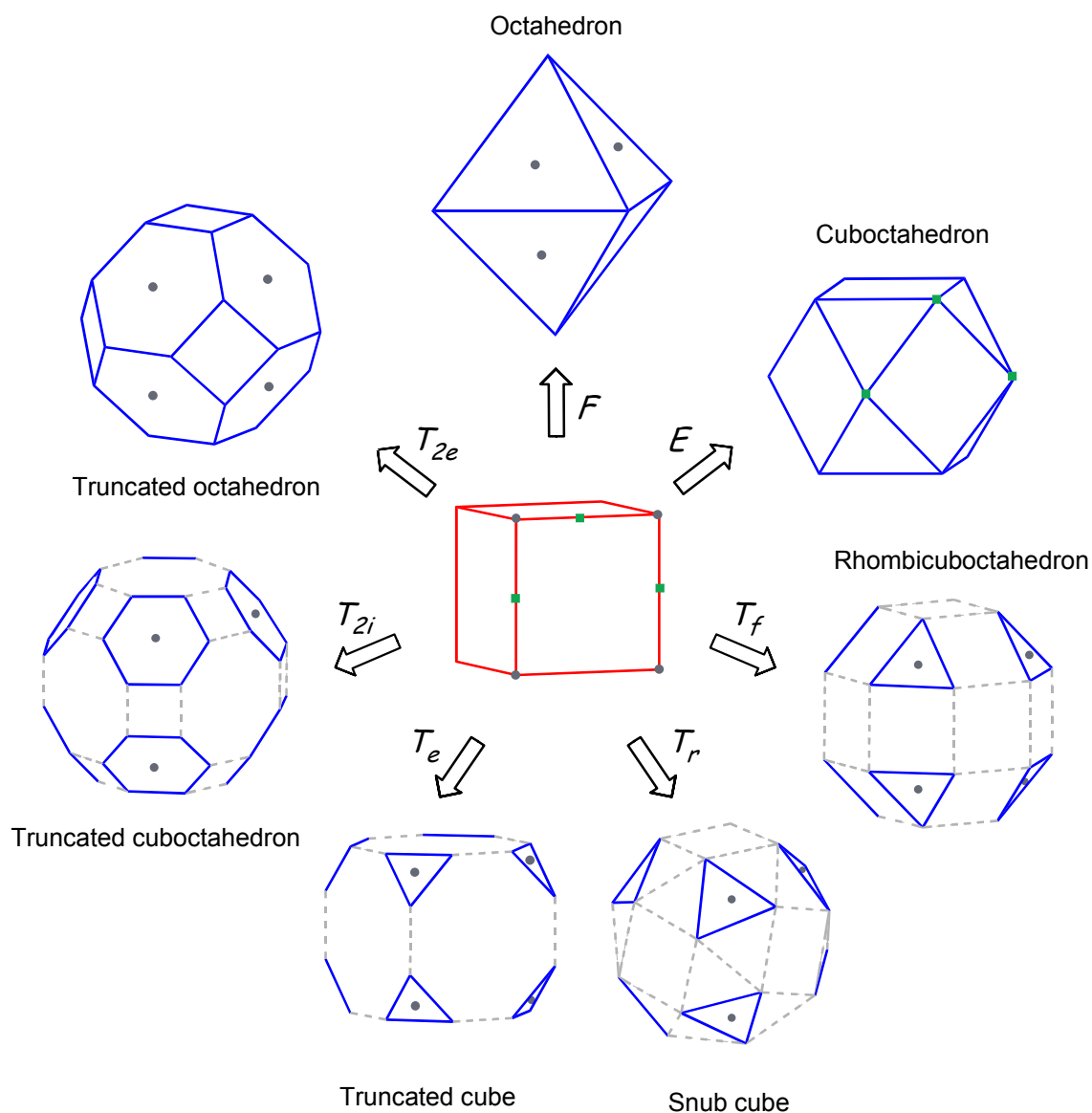
**Figure S2.** Polyhedra generated from a cube through the following operations: face augmentation $(A_F)$, edge augmentation $(A_E)$, face-directed truncation $(T_f)$, rotated truncation $(T_r)$, edge-directed truncation $(T_e)$, and two double truncations with independent hexagons $(T_{2i})$ and with edge-sharing octagons $(T_{2e})$. The correspondence between some vertices of the octahedron and the faces of the generated polyhedra are noted with gray dots, that between edges of the octahedron and vertices of the cuboctahedron with green squares.

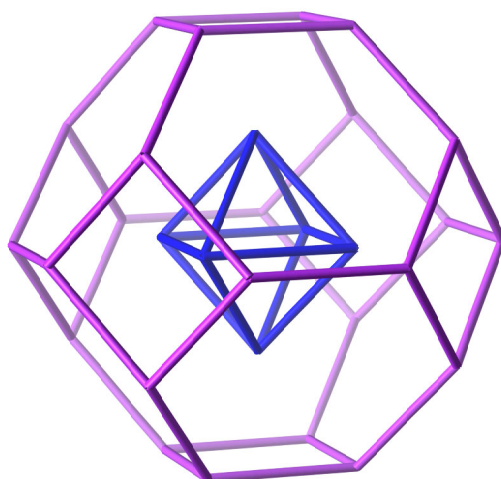**Figure S3.** Diamond shells 2 and 6 around centroid of adamantanoid unit, forming an octahedron and a truncated octahedron.