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T-symmetrical icosahedra: A new type of chirality in metal complexes

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Supporting Information

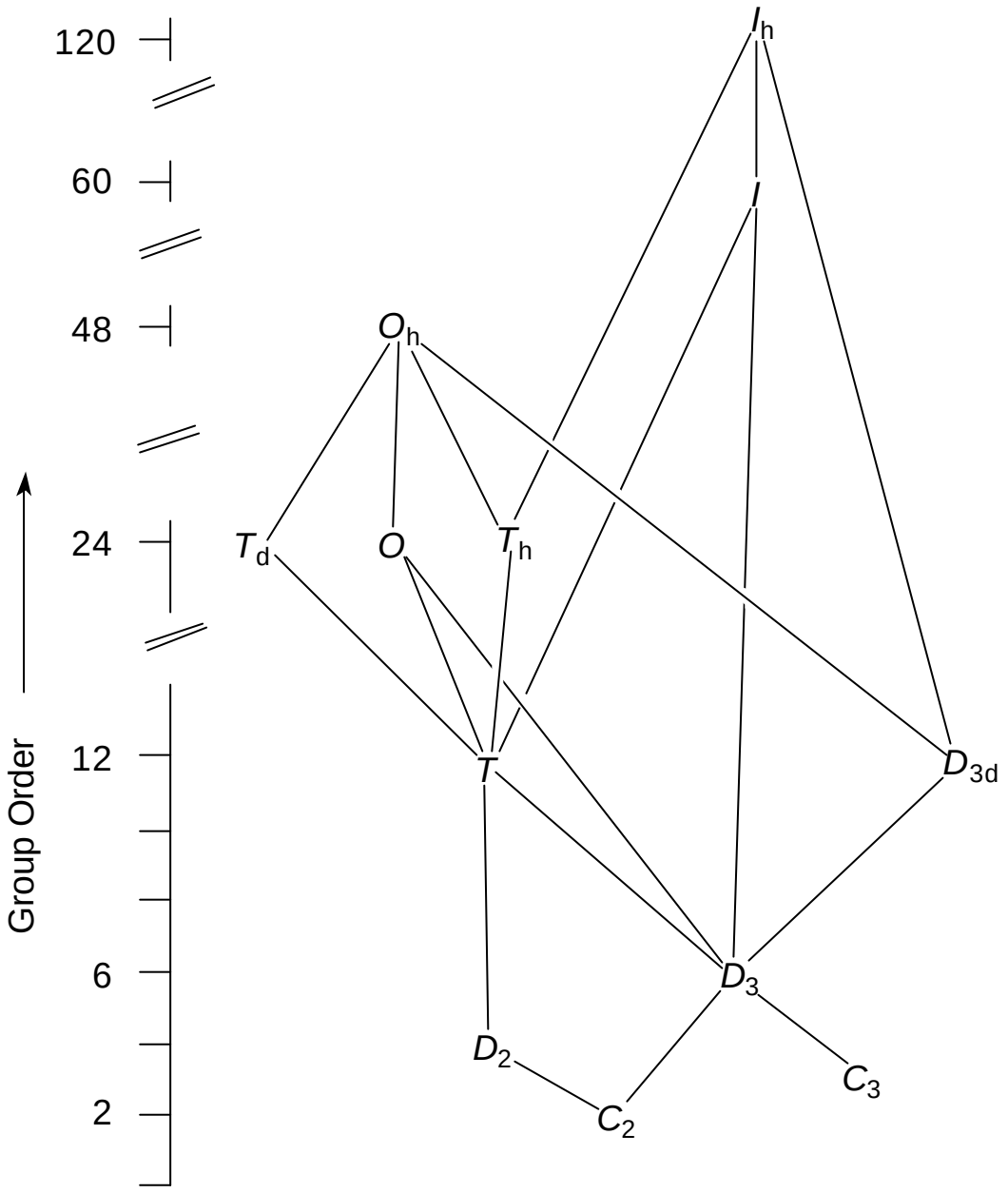


Figure S1. Correlation of some point groups discussed in the text. The five solutions of an icosahedron with six colored edges have T_h, D_{3d}, D_3, D_2, and C_2-symmetry. The solution with four colored triangles has T-symmetry.

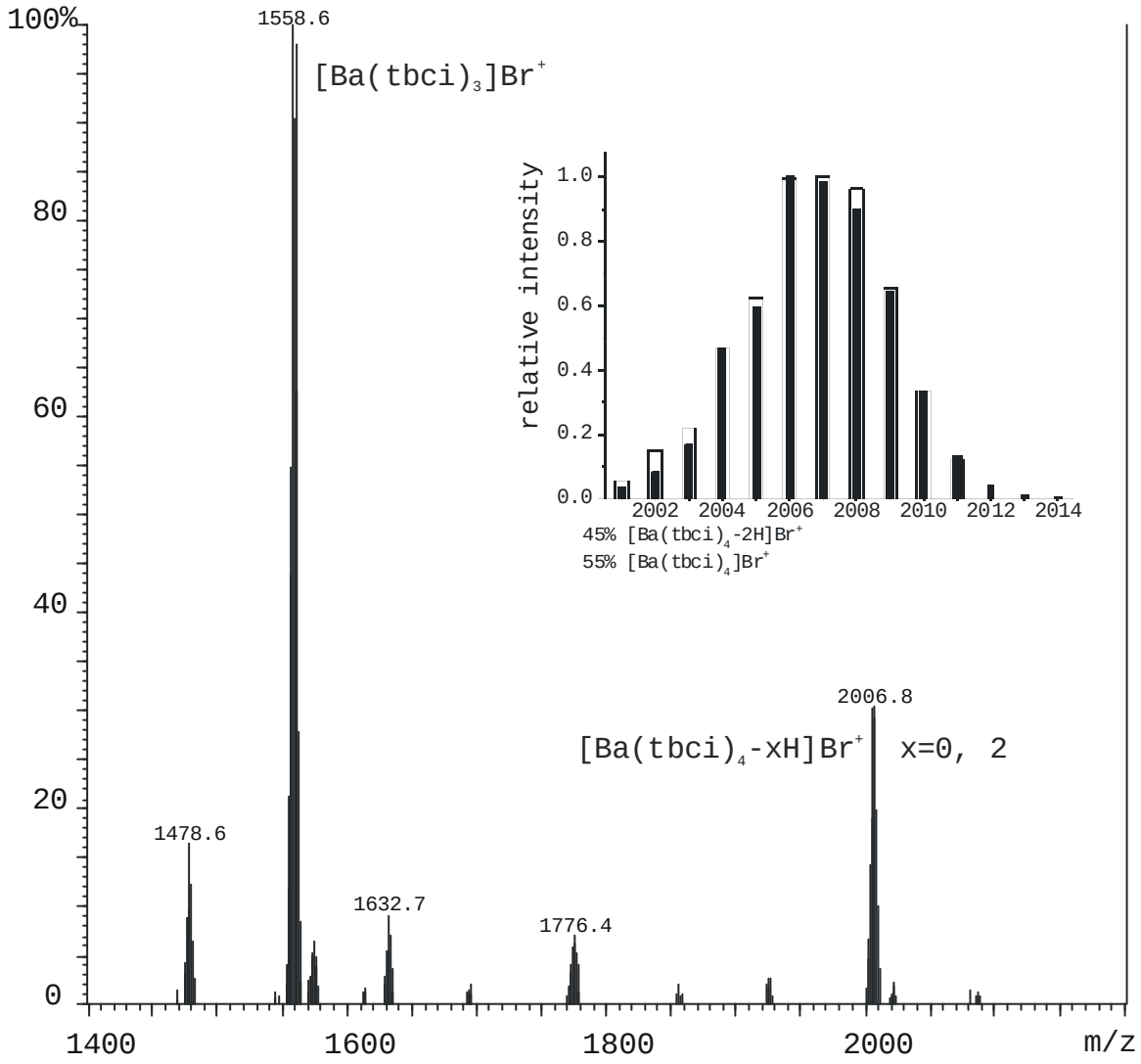


Figure S2. FAB^+ mass-spectrum of $[Ba(tbci)_4]Br_2$. The inlet shows the calculated (black columns) and measured (white columns) isotope pattern of the peak at m/z = 2006.8.

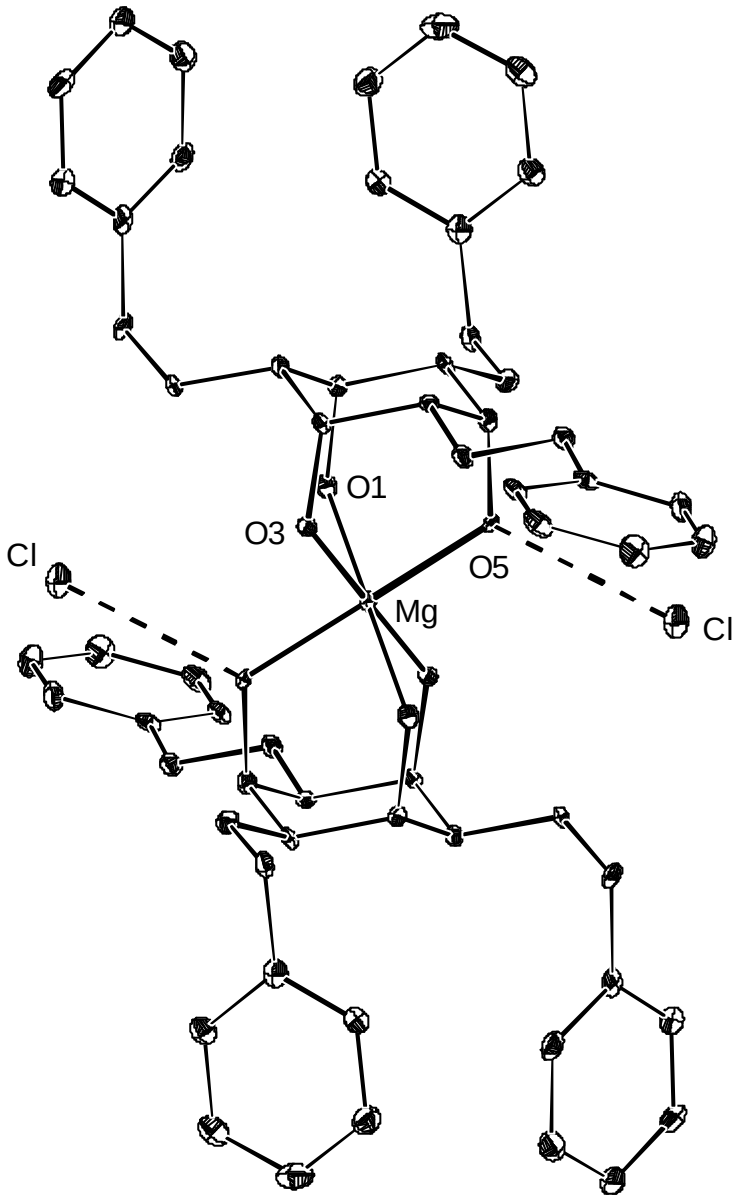
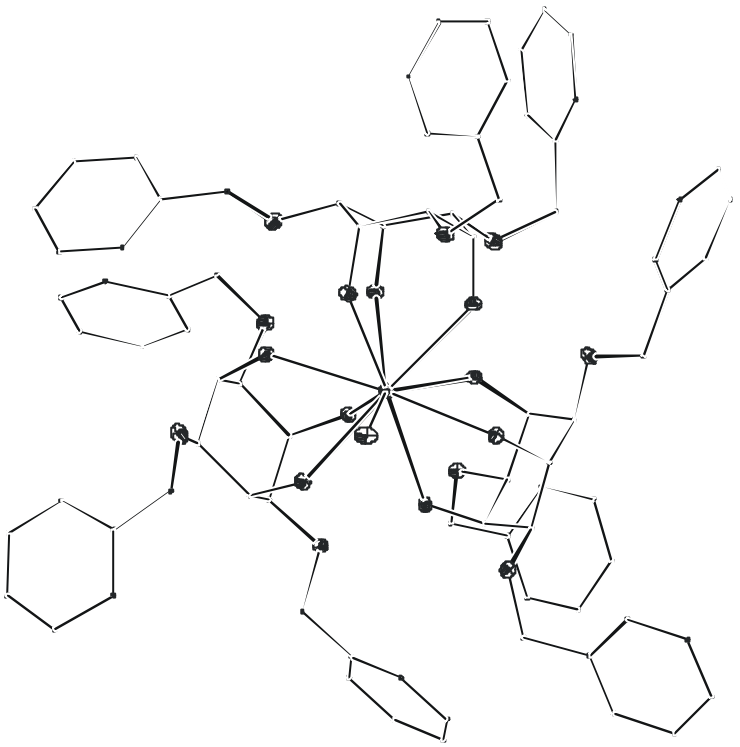


Figure S3. ORTEP-representation of $[Mg(tbci)_2]Cl_2$ with numbering scheme and vibrational ellipsoids at the 30% probability level. Hydrogen atoms are omitted for clarity.

a)



b)

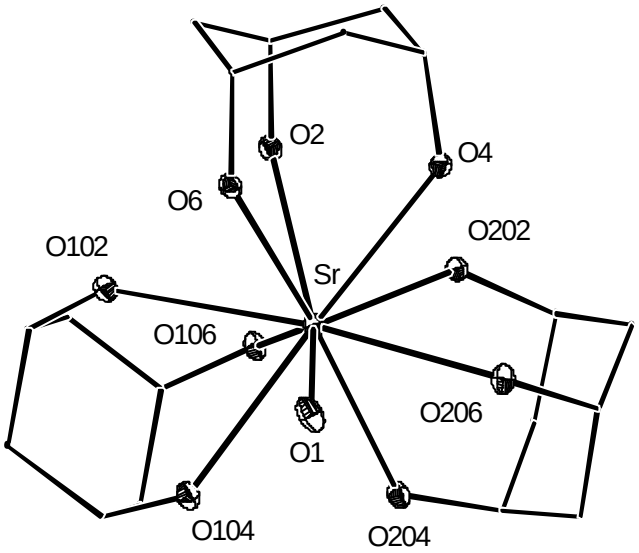


Figure S4. Structure of $[Sr(tbci)_3(OH_2)]^{2+}$: a) the entire complex cation; b) the complex core. The Sr center and the O- and N-atoms are shown as ellipsoids at the 30% probability level; the backbone of the ligands is represented by a stick model; hydrogen atoms are omitted for clarity.

Table S5 Survey of Hexanitrato-complexes

CCDC-Ref. code	Symmetry	Metal-Center
BAGFEU	T_h	Nd
BEQVAU	T_h	Th
CILKOX	T_h	Ce
COCYOI	D_3	Th
COKVAZ01	T_h	La
DEYDUG	T_h	Nd
FIBNAF	T_h	Nd
FIVCIW	D_3	La
GEZHIC	T_h	Nd
GEZHOI	T_h	Eu
GIGPOB	D_3	Np
GOBTAS	T_h	Th
HIRMEA	T_h	Ce
JIZSOA	D_3, T_h	La, La[a]
LAPKOC	D_3	La
MALMAN	D_3	La
NMPOTH	T_h	Th
PILPIJ	S_6	Pb[b]
PILPIJ10	D_3	Ba
PILPOP	D_3	Pb
SERWER	T_h	Eu
TINTUF	D_3	La
TUMWUT	D_3	La
VIJSAI	T_h	Th
VUYWOB	T_h	Gd
VUZDOJ	T_h	U[c]
WIDXAI	T_h	La
YAGFIV	T_h	La
YUWWAO	D_3	Th
ZEWBOS	T_h	Th
ZOBNOT	D_3	Ce

[a] Two different isomers in the same crystal structure

[b] Distorted cuboctahedron

[c] Some of the nitrato ligands are severely disordered

Crystal data of $[Mg(tbci)_2]Cl_2 \cdot 10MeOH$

Crystals of composition $[Mg(tbci)_2]Cl_2 \cdot 10MeOH$ disintegrate rapidly upon exposure to air. A crystal of dimensions 0.52 × 0.32 × 0.13 mm was therefore embedded in perfluorpolyether and data collection was performed at 100(2) K on a SIEMENS SMART-CCD diffractometer ($Mo_{K\alpha}$-radiation, l = 71.073 pm, graphite monochromator, μ = 0.168 mm^{-1}): space group $P\bar{1}$, a = 1097.95(9), b = 1223.9(1), c = 1409.3(1) pm, a = 87.41(2)°, b = 73.92(2)°, g = 75.08(2), Z = 1, V = 17577(3) × 10^6 pm^3, r_{calc} = 1.238 Mg m^{-3}. Numerical absorption correction (T_{min} = 0.457, T_{max} = 0.962). $2q_{max}$: 50.0°. Of 7451 measured reflections 5502 independent reflections were used for the refinement of 439 parameters, the structure was solved by direct methods (SHELXS-97). All non hydrogen atoms were refined with anisotropic displacement parameters (SHELXL-93, full-matrix least-squares calculations on F^2). H(-C)-atoms were placed at calculated positions (riding model). R [$F_o^2 > 2s(F_o^2)$]: 7.23%, wR_2 (all data): 19.28%. Residual electron density: +1.012 / -0.444 $e^o/Å^3$.

Crystal data of $[Sr(tbci)_3(OH_2)]Br_2 \cdot 4MeOH$

Crystals of composition $[Sr(tbci)_3(OH_2)]Br_2 \cdot 4MeOH$ disintegrate rapidly upon exposure to air. A crystal of dimensions 0.30 × 0.13 × 0.09 mm was therefore embedded in perfluorpolyether and data collection was performed at 100(2) K on a SIEMENS SMART-CCD diffractometer ($Mo_{K\alpha}$-radiation, l = 71.073 pm, graphite monochromator, μ = 1.645 mm^{-1}): space group $P\bar{1}$, a = 1505.20(9), b = 1581.42(9), c = 1941.1(1) pm, a = 101.36(1)°, b = 97.24(1)°, g = 107.24(1), Z = 2, V = 4241.7(5) × 10^6 pm^3, r_{calc} = 1.359 Mg m^{-3}, semi-empirical absorption correction (MulScanAbs, Platon99 program suite, A.L. Spek, Univ. Utrecht, Netherlands: T_{min} = 0.633, T_{max} = 0.719), $2q_{max}$: 60.0°. Of 42664 measured reflections 24651 independent reflections were used for the refinement of 1068 parameters, the structure was solved by direct methods (SHELXS-97). All nonhydrogen atoms were refined with anisotropic displacement parameters (SHELXL-93, full-matrix least-squares calculations on F^2). H(-C)-atoms were placed at calculated positions (riding model). H(-O) and H(-N) atoms were located from the difference map, distances of chemically equivalent H-atoms were restrained to be equal within errors (73 restraints). R [$F_o^2 > 2s$ (F_o^2)]: 5.40%, wR_2 (all data): 14.28%. Residual electron density: +1.549 / -1.048 $e^o/Å^3$.

Synthesis and Characterization of $[Sr(tbci)_3]Br_2 \cdot 4MeOH$

$SrBr_2 \cdot 6H_2O$ (25 mg) and tbci (100 mg) were dissolved in dry MeOH (5 mL) and allowed to stay for several days at 4°C. The resulting crystals (30 mg, 25%) disintegrated in air. Anal. Calc. for $C_{83}H_{107}N_9O_{11}Br_2Sr$: C, 60.26; H,6.52; N, 7.62. Found: C, 60.27; H, 6.42; N, 7.73. FAB^+-MS: m/z = 1511.0 (28.2%, $[Sr(tbci)_3Br]^+$).

Synthesis and Characterization of $[Mg(tbci)_2]Br_2 \cdot 10MeOH$

$MgCl_2 \cdot 6H_2O$ (25 mg) and tbci (100 mg) were dissolved dry MeOH (4 mL). The solution was kept at 4°C for several days. The resulting crystals (0.03g, 22%) decomposed very rapidly on air. Anal. Calc. for $C_{56.5}H_{81}N_6O_{11}Cl_2Mg$: C, 60.83; H, 7.32; N, 7.53. Found: C, 60.61, H, 7.31, N, 7.50. FAB^+-MS: m/z = 917.4 (43.4%, $[Mg(tbci)_2-H]^+$).

1,3,5-Tris(benzylamino)-1,3,5-trideoxy-*cis*-inositol (tbci)

Taci (1g, 5.6 mmol) was dissolved in dry MeOH (50 mL) and benzaldehyde (2.3 mL, 23.6 mmol) was added. The solution was stirred for 2 hours at 50°C. $NaBH_4$ (1.8 g, 47.6 mmol) was then added in portions. The mixture was stirred for 12 h and an additional portion of $NaBH_4$ (0.2g, 5.3 mmol) was added. Stirring was continued for 1 h. The pH was then adjusted to 1 (conc. HCl). A white precipitate formed which was filtered off, extracted with MeOH and discarded. The combined MeOH fractions were sorbed on Dowex 50 W X 2 (100-200 mesh) and the column was successively eluted with H_2O (400 mL), 1 M HCl (400 mL) and 8M HCl (1 L). The last fraction was evaporated to dryness, and the resulting white solid was dissolved in H_2O. The solution was alkalized with 1M KOH. The free tbci (white solid, 77 %) was isolated by filtration, washed with H_2O, and recrystallized from EtOH. Anal. Calc. for $C_{27}H_{33}N_3O_3$: C, 72.46; H, 7.43; N, 9.39. Found: C,72.66; H, 7.79; N,9.20. ^1H NMR ($CDCl_3$): δ= 7.32-7.21 (m,15 H), 4.03 (t, 3H), 3.86 (s,6 H), 2.37 (t,3 H). ^{13}C NMR ($CDCl_3$): δ= 140.0, 128.5, 128.2, 127.1, 70.2, 58.2, 50.7. FAB^+-MS: m/z = 448.1 (100%, $Htbci^+$).

1,3,5-Tris(benzyl-methyl-amino)-1,3,5-trideoxy-*cis*-inositol (tbmci)

tbci (0.5 g, 1.1 mmol) was dissolved in diluted formic acid (80 mL of conc. HCOOH, 20 mL of H_2O). Formaldehyde (12 mL of a 37 % aqueous solution) was then added and the mixture was refluxed for 14 h. After cooling to room temperature, conc. HCl (50 mL) was added and the solution was evaporated to dryness in vacuo. The residue was dissolved in H_2O and alkalized with 1M aqueous KOH. The suspension was extracted with chloroform (4 x 100 mL), and the combined $CHCl_3$-fractions were evaporated to dryness. The residue was dissolved MeOH (5 mL) and allowed to stay at 4°C. Free tbmci crystallized as white needles (60 %). Anal. Calc. For $C_{30}H_{39}N_3O_3$: C, 73.59; H, 8.03; N, 8.58. Found: C, 73.82; H, 7.95; N, 8.54. ^1H NMR ($CDCl_3$): δ= 7.35-7.25 (m, 15 H), 4.62 (t, 3H), 3.89 (s, 6H), 2.47 (s, 9H), 2.20 (t, 3H). ^{13}C NMR ($CDCl_3$): δ= 139.0, 128.9, 128.3, 127.0, 67.7, 65.5, 58.5, 39.3. FAB^+-MS: m/z = 490.3 (100%, $Htbmci^+$).

On Special Colourings of an Icosahedron

An icosahedron is a polyhedron of type (3; 5), that means the faces are triangles and five faces meet in each corner.
By an **admissible colouring** we mean: there are as much coloured edges as possible, but two coloured edges do not have a common corner. Two colourings C and C' are **inequivalent**, if we cannot transform C to C' by rotations or reflections and rotations.

1. The icosahedron and its stabilizer

Definition. Fix an icosahedron $\mathcal{I}$ in $\mathbb{R}^3$ with barycenter O, the origin of $\mathbb{R}^3$.
(i) Over $\mathbb{R}^3$ we have the group of isometries, that is, of linear maps which fix the point O. In general one distinguishes the two groups

$O(3)$:= {isometries of $\mathbb{R}^3$ }
= {combinations of rotations and reflections with fixed point O}
$SO(3)$:= {combinations of rotations with fixed point O}$\subset O(3)$.

One says that $O(3)$ and $SO(3)$ act on $\mathbb{R}^3$.
(ii) Considering a subset M $\subset \mathbb{R}^3$ and a subgroup $G \subset O(3)$ we can decide for an element $s \in G$ whether $s(M) \neq M$ or $s(M) = M$. In the second case we call s an element of the stabilizer $Stab_G(M)$ of M with respect to G. For each $s \in G$ the set $s(M)$ is said to be equivalent to M with respect to G or M and $s(M)$ lie in the same orbit.
(iii) For the icosahedron $\mathcal{I}$ with barycenter O we define $\mathbb{I}$:= $Stab_{SO(3)}$ ($\mathcal{I}$) and $\mathbb{I}^*$:= $Stab_{O(3)}$ ($\mathcal{I}$):
For general definitions of action, stabilizer and so on, see [S1, section 1.6].

1.1. Number of coloured edges.

It is clear that a colouring is admissble if each corner has exactly one coloured edge. Each edge has exactly two corners and the whole icosahedron has twelve corners. Therefore we decompose the set of twelve corners in pairwise distinct subsets with two corners. In this way we get 6 = $\frac{12}{2}$ subsets with two elements and so every admissible colouring has at most six couloured edges. Below we will see that such admissible colourings exist.

1.2. Description of $\mathbb{I}$.

First we characterize the elements of $\mathbb{I}$. Let

R_5 := {rotation around lines through two opposite corners with angle $\frac{2k}{5}p$ and 1 ≤ k ≤ 4 },

R_3 := {rotation around lines through midpoints of two opposite faces with angle $\frac{2k}{3}p$ and 1 ≤ k ≤ 2},

R_2 := {rotation around lines through midpoints of two opposite edges with angle p },

then we have $\mathbb{I} = R_5 \cup R_3 \cup R_2 \cup \{id\}$. Here an element $r \in R_5$ has order[1] 5, any $s \in$ R3 has order 3 and any $t \in R_2$ has order 2. By a suitable choice of $s \in R_3$ and $t \in R_2$ we get a complete description of $\mathbb{I}$ with generators and relations (see [S1, section2.2]):

$$\mathbb{I} = \langle s, t \mid s^3 = t^2 = (st)^5 = id \rangle$$

This means, each element of $\mathbb{I}$ may be written as the composite of a certain number of s's and t's (a "word in s and t") and the conditions $s^3 = t^2 = (st)^5 = id$: are fulfilled.
For example $s^3ts^2t^2$ is a word in s and t , which is the same as s^2t. Therefore $\mathbb{I}$ is isomorphic[2] to A_5, the subgroup of all even permutations of S_5, the group of all permutations of {1, 2, 3, 4, 5}. It is well known that this group has $60 = \frac{5!}{2}$ elements (see [S2, page 2] and [S1, section 1.2]).
If we consider reflections as symmetries too, then it is enough to choose the point symmetry p_0 as a supplementary generator, because each reflection is a product of p_0 with a suitable rotation. Therefore the stabilizer of $\mathcal{J}$ with respect to $O(3)$ has the form:

$\mathbb{I}^* = \mathbb{I} \cup p_0 \mathbb{I} = A_5$ X Z/2 Z (see [S3, section 12.5]).

Let now C be the set of all admissible colourings C of $\mathcal{J}$. Then we find that $\mathbb{I}$ and $\mathbb{I}^*$ respectively, act on C. If an element of $SO(3)$ or $O(3)$, fixes a colouring, it lies already in $\mathbb{I}$ or $\mathbb{I}^*$, respectively. Therefore we restrict our considerations to $\mathbb{I}$ or $\mathbb{I}^*$.

.
Two colourings C and C' are equivalent with respect to $\mathbb{I}$ (or $\mathbb{I}^*$)if there exists a $s \in \mathbb{I}$ (or $s \in \mathbb{I}^*$) with $s(C) = C'$. To determine the number of orbits with respect to $\mathbb{I}$ (and consequently the number of inequivalent colourings), we use a connection between the cardinalities of orbits, stabilizers and C:

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[1] Let G be finite group. The *order* of an element g ∈ G is the least integer $k > 0$ with $g^k = id$.

[2] The group $\mathbb{I}$ has the same structure, therefore it is almost the same as A_5.

(1) $$\#(\mathcal{C}) = \sum_{C} \frac{\#(\Pi)}{\#\,\mathrm{Stab}_{\Pi}(\mathcal{C})}$$

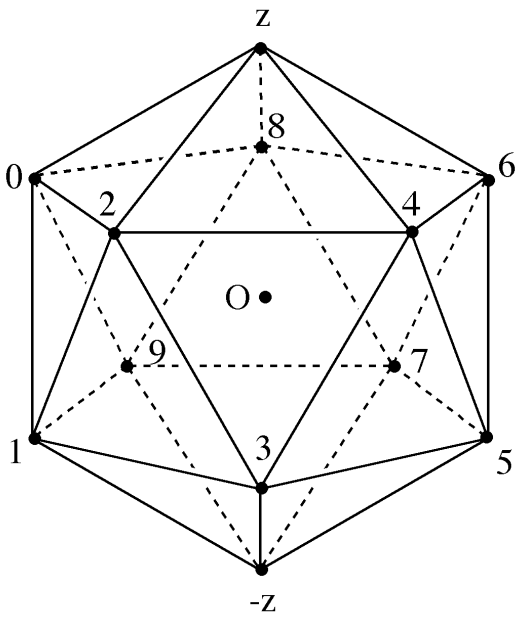
where C runs over a set of representations of admissible colourings[3] (see [S1, section 1.6]).

2. SKETCH FOR THE STRATEGY FOR SOLUTION

Now we label the corners of the icosahedron $\mathcal{I}$. Then we describe all axes of the elements of Π unambignously by the corners, edges and triangles, respectively, which meet the axis. Moreover we can list all colourings of $\mathcal{I}$. In the next step we select eight colourings and show that these are inequivalent. At last we use (1) to show that these are all inequivalent colourings.

3. LABELLING

We mark two opposite corners -like a North and a South Pole- and call them z and $-z$.
Then we label all corners which are adjacent to z (this means there is an edge between this corner and z) with the even numbers 0, 2, 4, 6, 8 and the neighbours of $-z$ with the odd numbers 1, 3, 5, 7, 9. Thereby we pay attention that the corners of each triangle "of the middle" are successive numbers.



[3] $\#G$:= cardinality of G

Now we can describe each edge by a pair of labels (namely the labels of its corners). We get that the pair (x, y) of labels describe an edge if

(i) $(x, y) = (z, i)$ with i is even and $0 \le i \le 8$
or
(ii) $(x, y) = (i, -z)$with i is odd and $1 \le i \le 9$
or
(iii) $(x, y) = (i, j)$with $i-j \equiv 1, 2, 8$ or 9 (mod 10)[4] and $0 \le i < j \le 9$

An analogous description with triples yields for the triangles.
Now for rotation axes we have the following description (the symbol $\leftrightarrow$ means that these are the two opposite corners, edges or triangles which meet the axis):

$$\{i \leftrightarrow i+5 \quad 0 \le i \le 4\} \cup \{z \leftrightarrow -z\} \quad \rightarrow R_5$$

$$\left.\begin{array}{l}\{(i, i+1, i+2) \leftrightarrow (i+5, i+6, i+7) \mid 0 \le i \le 4\} \\ \{(2i, 2i+2, z) \leftrightarrow (2i+5, 2i+7, -z) \mid 0 \le i \le 4\}\end{array}\right\} \rightarrow R_3$$

$$\left.\begin{array}{l}\{(i, i+1) \leftrightarrow (i+5, i+6) \mid 0 \le i \le 4\} \\ \{(i, i+2) \leftrightarrow (i+5, i+7) \mid 0 \le i \le 4\} \\ \{(2i, z) \leftrightarrow (2i+5, -z) \mid 0 \le i \le 4\}\end{array}\right\} \rightarrow R_2$$

For example: if $r \in R_5$ is a rotation with angle $\frac{2}{5}p$ and axis $z \leftrightarrow -z$, then $r_0(i) = i + 2$.
Finally the point symmetry has now the form $r_0(i) \equiv i + 5$ (mod 10) for all i and $r_0(z) = -z$.

4. COLOURINGS

To describe all admissible colourings we use a decision tree. Each vertex of the tree means a coloured edge, only admissible colourings are mentioned. We follow a lexicographical ordering in two ways: each pair is ordered and from each vertex to the next we take the next corner of the icosahedron which has no coloured edge. Since each corner has exactly one coloured edge we can start in z without loss of generality. Then we can colour the five edges

[4] "(mod 10)" is a special way of calculation. Here it is enough to "forget the ten's places", e.g.: $14 \equiv 4$(mod 10) or 5+7 =12 and 5+7 $\equiv$2 (mod 10).

$(z, 0), (z, 2), (z, 4), (z, 6), (z, 8).$

Each choice gives us the same tree structure. Therefore we only consider $(z,0)$ and multiply our result with 5. Now for the next vertex we have four possibilities:

$$(1, 2); (1, 3); (1, 9); (1, -z):$$

In the figures S7 to S9 we show the different subtrees. Altogether we have 25 colourings if $(z, 0)$ is coloured and therefore we get $\#\mathscr{C} = 125$.

5. INEQUIVALENT COLOURINGS

Now we look at the set of colourings $\mathscr{R} = \{T_h, D_{3d}, D_2, \overline{D_2}, D_3, \overline{D_3}, C_2, \overline{C_2}\}$ with coloured edges

$$
\begin{array}{ll}
T_h: & (z,0),\ (1,9),(2,3),\ (4,6),(5,-z),\ (7,8), \\
D_{3d}: & (z,0),\ (1,3),(2,4),(5,-z),\ (6,8),\ (7,9), \\
D_2: & (z,0),(1,-z),(2,4),\ (3,5),\ (6,8),\ (7,9), \\
\overline{D_2}: & (z,6),\ (0,8),(1,3),\ (2,4),(5,-z),\ (7,9), \\
D_3: & (z,0),\ (1,2),(3,5),\ (4,6),\ (7,8),(9,-z), \\
\overline{D_3}: & (z,4),\ (0,8),(1,9),\ (2,3),(5,-z),\ (6,7), \\
C_2: & (z,0),\ (1,9),(2,4),\ (3,5),\ (6,8),(7,-z), \\
\overline{C_2}: & (z,2),\ (0,8),(1,3),\ (4,6),(5,-z),\ (7,9),
\end{array}
\tag{2}
$$

In figure S10 we illustrate these colourings. First we calculate the cardinality of the stabilizer of each element of $\mathscr{R}$ with respect to $\mathbb{II}$.

5.1. Rotation of order 5. In general an isometry $r \in \mathbb{II}$ is a symmetry of a colouring C if and only if each coloured edge is mapped by r to a coloured edge. From this point of view we see immediately that $R_5 \cap Stab_{\mathbb{II}}(C) = \emptyset$ because exactly two opposite corners are fixed by an element of R_5.

5.2. Rotation of order 3. What are the conditions on a $s \in R_3$ and a colouring $C \in \mathscr{C}$ to meet $s \in Stab_{\mathbb{II}}(C)$? If s is a symmetry, then it has to fix two triangles with uncoloured edges. Moreover the coloured edges which emanate from each corner of the triangle must be in the same relative position. So we find out:
Let s be a rotation about the barycenter of the triangles $(i, i+1, i+2) \leftrightarrow (i+5, i+6, i+7)$. Then $s \in Stab_{\mathbb{II}}(C)$ if and only if C has one of the following colourings:

- $(i, i+8),\ (i+1, \mp z),\ (i+2, i+4),\ (i+3, i+5),\ (i+6, \pm z),\ (i+7, i+9)$ or
- $(i, i+9),\ (i+1, i+3),\ (i+2, \pm z),\ (i+4, i+5),\ (i+6, i+8),\ (i+7, \mp z)$ or
- $(i, i+9),\ (i+1, i+3),\ (i+2, \pm z),\ (i+4, i+6),\ (i+5, \mp z),\ (i+7, i+8)$ or
- $(i+9, i+1),\ (i+2, i+3),\ (i, \mp z),\ (i+4, i+5),\ (i+6, i+8),\ (i+7, \mp z)$ or
- $(i+9, i+1),\ (i+2, i+3),\ (i, \mp z),\ (i+4, i+6),\ (i+5, \mp z),\ (i+7, i+8)$,

Table S2

	axes through the midpoint of		
	triangles	edges	$p_O \in \mathrm{Stab}_{\Pi^*}(.)$?
T_h	$(z,2,4) \leftrightarrow (7,9,-z)$ $(z,6,8) \leftrightarrow (1,3,-z)$ $(0,1,2) \leftrightarrow (5,6,7)$ $(0,8,9) \leftrightarrow (3,4,5)$	$(z,0) \leftrightarrow (5,-z)$ $(1,9) \leftrightarrow (4,6)$ $(2,3) \leftrightarrow (7,8)$	*yes*
D_{3d}	$(0,1,9) \leftrightarrow (4,5,6)$	$(z,2) \leftrightarrow (7,-z)$ $(z,8) \leftrightarrow (3,-z)$ $(2,3) \leftrightarrow (7,8)$	*yes*
D_2		$(z,8) \leftrightarrow (3,-z)$ $(0,1) \leftrightarrow (5,6)$ $(2,4) \leftrightarrow (7,9)$	*no*
$\overline{D_2}$		$(z,8) \leftrightarrow (3,-z)$ $(0,1) \leftrightarrow (5,6)$ $(2,4) \leftrightarrow (7,9)$	*no*
D_3	$(z,6,8) \leftrightarrow (1,3,-z)$	$(0,2) \leftrightarrow (5,7)$ $(0,9) \leftrightarrow (4,5)$ $(2,4) \leftrightarrow (7,9)$	*no*
$\overline{D_3}$	$(z,6,8) \leftrightarrow (1,3,-z)$	$(0,2) \leftrightarrow (5,7)$ $(0,9) \leftrightarrow (4,5)$ $(2,4) \leftrightarrow (7,9)$	*no*
C_2		$(3,4) \leftrightarrow (8,9)$	*no*
$\overline{C_2}$		$(3,4) \leftrightarrow (8,9)$	*no*

where we calculate (mod 10) and consider z if $2 \mid i$ and $-z$ otherwise. It is easy to check this.
If z is one of the corners of a triangle we get an analogous result.
Moreover we get for a $s \in R_3$: whenever $s \in \mathit{Stab}_{\Pi}(C)$ for a colouring C, then $s^2 \in \mathit{Stab}_{\Pi}(C)$ too.
Consequently: to count the elements of $\mathit{Stab}_{\Pi}(C) \cap R_3$, it is enough to count the symmetry axes, thus the corresponding pairs of opposite triangles, and to multiply this number with 2.

5.3. Rotation of order 2. We use the same way to decide whether $t \in R_2 \cap \mathit{Stab}_{\Pi}(C)$.
Here we have more possibilities for colourings if we start with a $t \in R_2$.
In figure S9 we give an example for $(i, i+1) \leftrightarrow (i+5;\ i+6) \rightarrow t$ and one colouring C.

In the same way all other combinations (t, C) with $t \in R_2 \cap Stab_{II}(C)$ can be determined.
Now we use these insights for our colourings in (2). The results are resumed in table S2.
With the formulas for each row in table S2:

$$\#Stab_{II}(.) = \#(Stab_{II}(C) \cap R_3) + \#(Stab_{II}(C) \cap R_1) + \#\{id.\}$$
$$= 2 \cdot \#\{\text{triangles}\} + \#\{\text{edges}\} + 1$$

$$\#Stab_{II^*}(.) = 2^k \cdot \#Stab_{II}(.) \text{ where } k = \begin{cases} 1 \text{ if } p_0 \in Stab_{II^*}(.) \\ 0 \text{ otherwise,} \end{cases}$$

we get the cardinalities of all stabilizers we are interested in. For example: T_h has four symmetry axes through barycenters of triangles. This gives us 8 = 2·4 elements of $Stab_{II}(T_h)$. Furthermore there are three symmetry axes through midpoint of edges. Thus we get three further elements of $Stab_{II}(T_h)$. Now we need still the identity $id.$, then the group $\mathrm{Stab}_{II}(T_h)$ is complete and we get $Stab_{II}(T_h)$=2·4+3+1 = 12. Since p_0 is a symmetry of T_h, we get $\#Stab_{II^*}(T_h)$=2·$Stab_{II}(T_h)$= 24. The results are collected in table S3.

Table S3

$\#\mathrm{Stab}_{\mathrm{II}}(T_h) = 2 \cdot 4 + 3 + 1 = 12$	$\#\mathrm{Stab}_{\mathrm{II}^*}(T_h) = 2 \cdot 12 = 24$
$\#\mathrm{Stab}_{\mathrm{II}}(D_{3d}) = 2 \cdot 1 + 3 + 1 = 6$	$\#\mathrm{Stab}_{\mathrm{II}^*}(D_{3d}) = 2 \cdot 6 = 12$
$\#\mathrm{Stab}_{\mathrm{II}}(D_2) = 2 \cdot 0 + 3 + 1 = 4$	$\#\mathrm{Stab}_{\mathrm{II}^*}(D_2) = 4$
$\#\mathrm{Stab}_{\mathrm{II}}(\overline{D_2}) = 2 \cdot 0 + 3 + 1 = 4$	$\#\mathrm{Stab}_{\mathrm{II}^*}(\overline{D_2}) = 4$
$\#\mathrm{Stab}_{\mathrm{II}}(D_3) = 2 \cdot 1 + 3 + 1 = 6$	$\#\mathrm{Stab}_{\mathrm{II}^*}(D_3) = 6$
$\#\mathrm{Stab}_{\mathrm{II}}(\overline{D_3}) = 2 \cdot 1 + 3 + 1 = 6$	$\#\mathrm{Stab}_{\mathrm{II}^*}(\overline{D_3}) = 6$
$\#\mathrm{Stab}_{\mathrm{II}}(C_2) = 2 \cdot 0 + 1 + 1 = 2$	$\#\mathrm{Stab}_{\mathrm{II}^*}(D_2) = 2$
$\#\mathrm{Stab}_{\mathrm{II}}(\overline{C_2}) = 2 \cdot 0 + 1 + 1 = 2$	$\#\mathrm{Stab}_{\mathrm{II}^*}(\overline{D_2}) = 2$

Since equivalent colourings have the same stabilizer there are obviously only three pairs which can be equivalent, namely (D_2, $\overline{D_2}$), (D_3, $\overline{D_3}$) and (C_2, $\overline{C_2}$). It is easy to see that $p_0(D_2) = \overline{D_2}$, $p_0(D_3) = \overline{D_3}$, and $p_0(C_2) = \overline{C_2}$ (see (2) and figure S10). Therefore they are equivalent with respect to $\mathbf{II}^*$, but not with respect to $\mathbf{II}$.

Because of

$$\sum_{C\in\mathcal{R}} \frac{\#\,II}{\#\,Stab(C)} = \frac{60}{12} = \frac{60}{6}+\frac{60}{4}+\frac{60}{4}+\frac{60}{6}+\frac{60}{6}+\frac{60}{2}+\frac{60}{2} = 125 = \#\mathcal{C}$$

we know that $\mathcal{R}$ consists exactly of all inequivalent colourings, if only rotations are allowed. If we consider the colourings with respect to $\mathbb{I}^*$ we get that all colourings are equivalent to T_h , D_{3d}, D_2, D_3 or C_2.

6. SUMMARY OF THE RESULTS

An admissible colouring of an icosahedron has precisley six coloured edges. There are eight inequivalent colourings, if we only allowed rotations of the icosahedron, and five colourings, if we can use reflections and rotations.

REFERENCES

[S1] Robinson, D.J.S.: A Course in the Theory of Groups, Springer. New York 1980
[S2] Conway, J.: Atlas of Finite Groups, Oxford University Press. 1985
[S3] Berger, M.: Geometry II, Springer. Berlin 1980

7. FIGURES

Figure S5

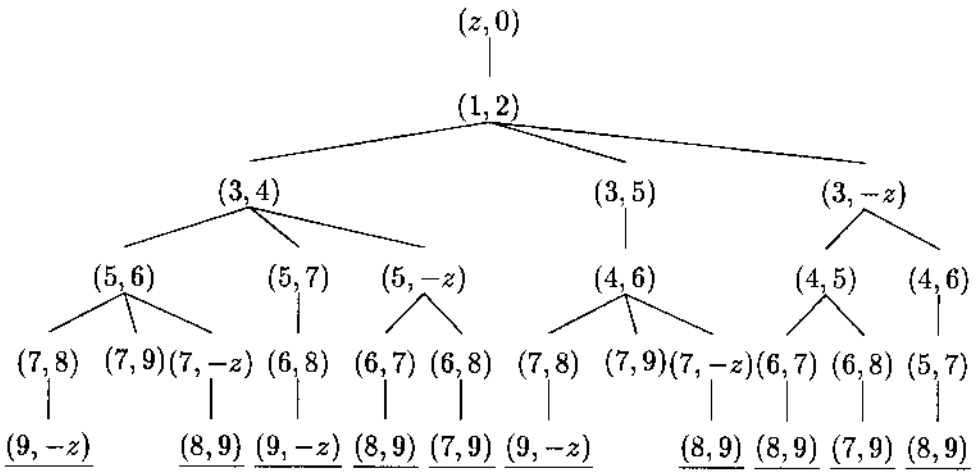


Figure S6

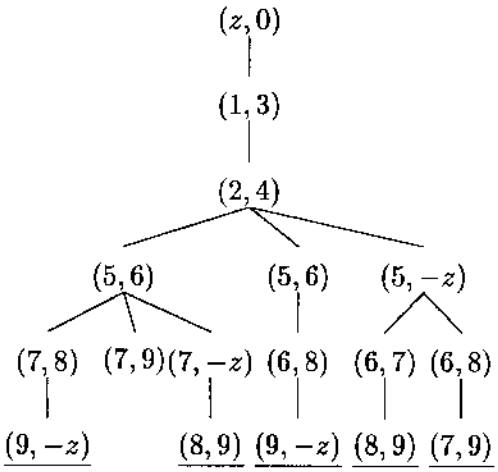


Figure S7

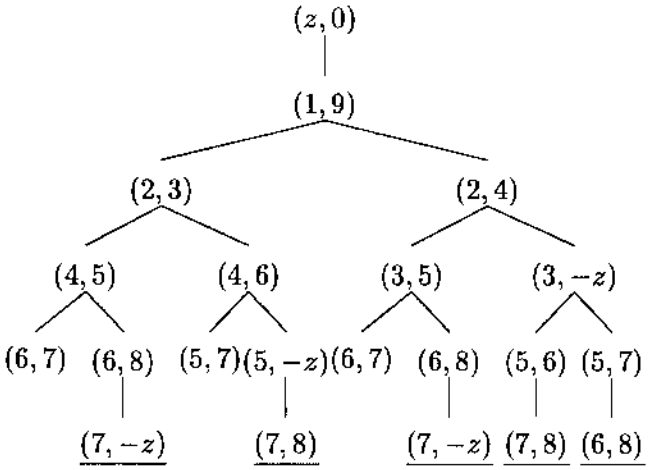


Figure S8

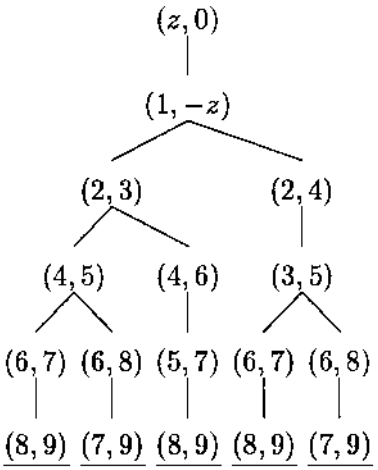


Figure S9

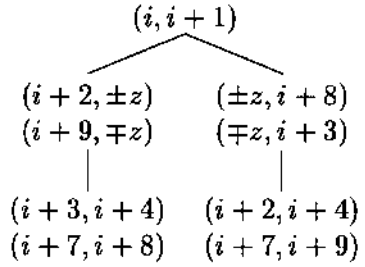
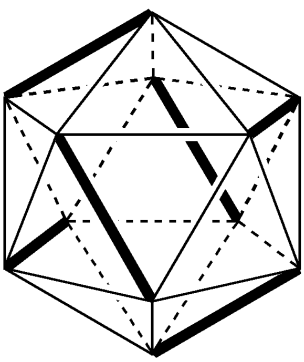
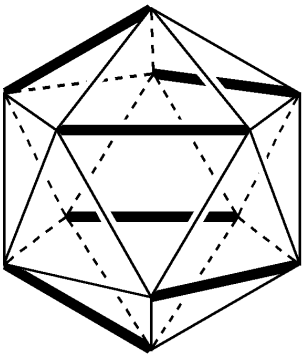


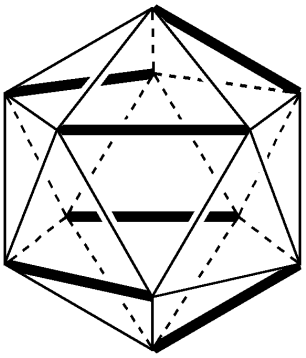
Figure S10. Inequivalent Configurations



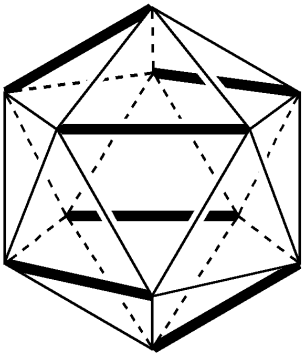
a) T_h



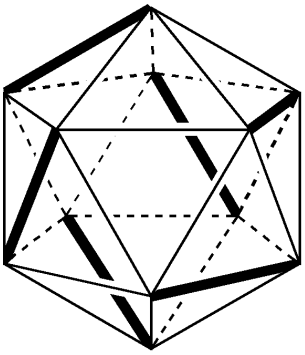
b) D_2



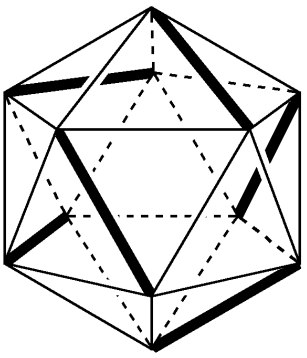
c) $\overline{D}_2$



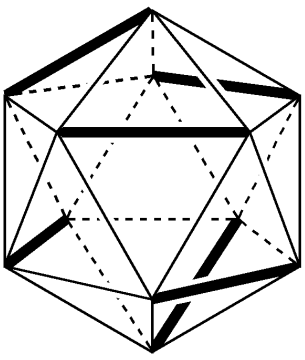
d) D_{3d}



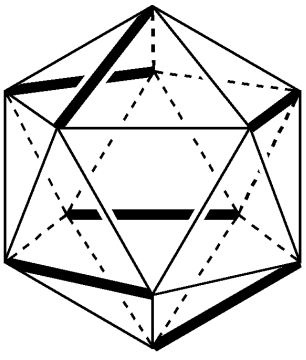
e) D_3



f) $\overline{D}_3$



g) C_2



h) $\overline{C}_2$