

A relation between vertex and edge orbits in nut graphs

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Rijeka, July 6, 2023

Rijeka Conference on Combinatorial Objects and their Applications



Inštitut za matematiko, fiziko in mehaniko

Spectra of graphs

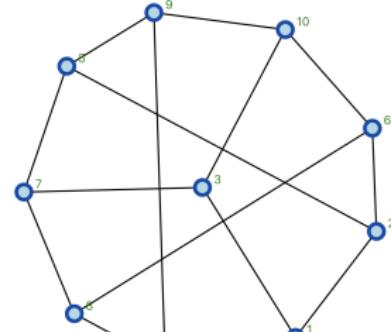
Let G be a finite simple graph of order n with the vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and let $E(G)$ denote the edge set of G .

The **adjacency matrix** of G is the matrix $A(G) = [a_{ij}]_{i,j=1}^n$, where

$$a_{ij} = a_{ji} = \begin{cases} 1 & \text{if } v_i v_j \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

Example:

$$A(\text{GP}(5, 2)) = \begin{bmatrix} 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \end{bmatrix}$$



Spectra of graphs

The **spectrum** of G , denoted $\sigma(G)$, is the multiset of eigenvalues of $A(G)$.

Examples:

$$\sigma(\text{GP}(5, 2)) = \{3, 1^5, (-2)^4\}$$

$$\sigma(K_{3,3}) = \{3, 0^4, -3\}$$

The exponents above give **multiplicity** of the eigenvalue, e.g. -2 is an eigenvalue of multiplicity 4 in $A(\text{GP}(5, 2))$. The multiplicity of the 0 eigenvalue is called **nullity** and denoted $\eta(G)$.

The eigenvalues are often ordered in non-increasing order

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n.$$

Graphs G and G' are called **cospectral** if $\sigma(G) = \sigma(G')$.

Singular and core graphs

A graph G is a **singular graph** if it has a zero eigenvalue.

The graph $K_{3,3}$ is singular, the graph $GP(5, 2)$ is non-singular.

A special class of singular graphs consists of the **core graphs**, graphs of which the kernel of the adjacency matrix contains a **full vector**. A full vector is a vector with no zero entry.

For example, the **kernel** (also called **null space**) of $A(K_{3,3})$ is

$$\ker A(K_{3,3}) = \text{span} \left\{ \mathbf{v}_1 = \begin{bmatrix} 1 \\ 0 \\ -1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \mathbf{v}_2 = \begin{bmatrix} 0 \\ 1 \\ -1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \mathbf{v}_3 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ -1 \end{bmatrix}, \mathbf{v}_4 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \right\}.$$

The local condition

An eigenvector \mathbf{v} can be viewed as a weighting of vertices, i.e. a mapping $\mathbf{v}: V(G) \rightarrow \mathbb{R}$.

A vector $\mathbf{v} \in \ker A$ if and only if for each vertex $v \in V(G)$ the sum of entries over the open neighbourhood $N_G(v)$ equals 0:

$$\sum_{u \in N_G(v)} \mathbf{v}(u) = 0$$

The above equation is called the **local condition**.

Example ($K_{3,3}$):

Nut graphs

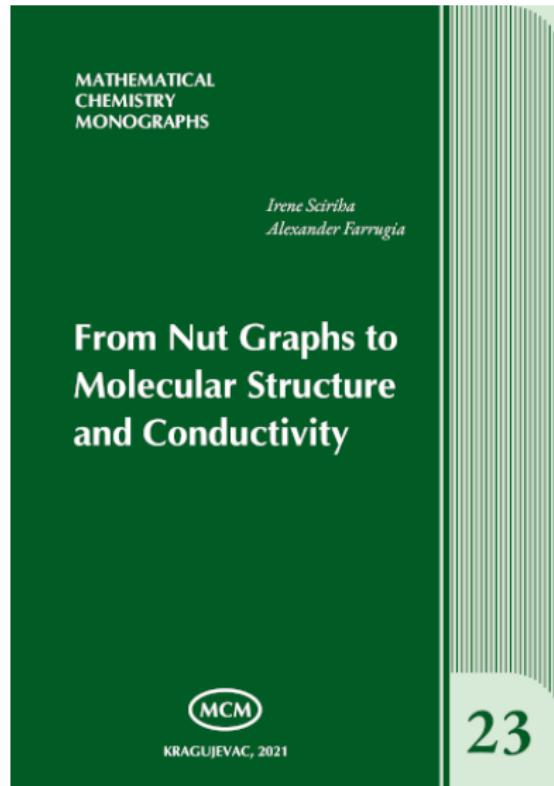
A simple graph G is a **nut graph** if G is a singular graph in which every non-zero vector in the kernel of $A(G)$ is full.

The term **nut graph** was coined in 1998 by Ivan Gutman and Irene Sciriha.

Here is an alternative (and, of course, equivalent) definition:

A simple graph G is a **nut graph** if G is a core graph with $\eta(G) = 1$.

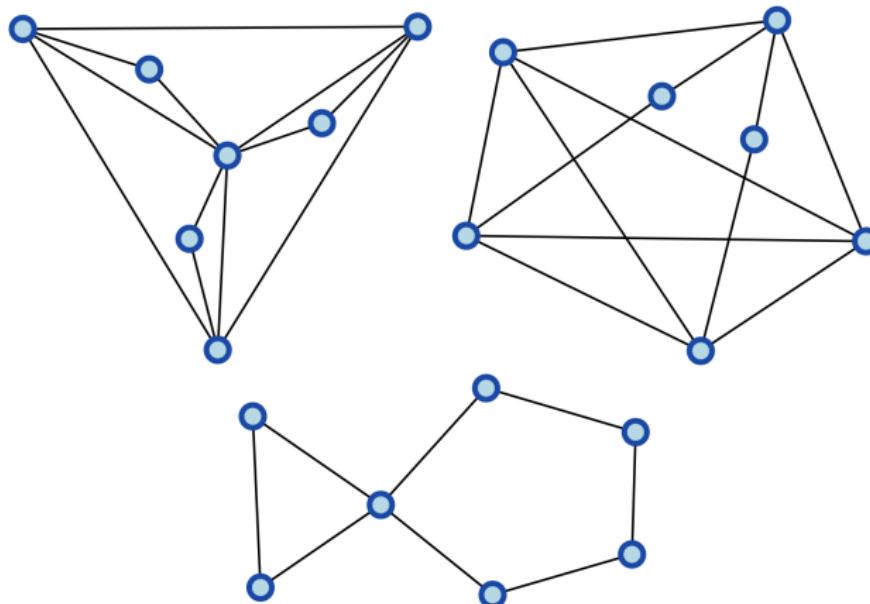
Why nut graphs?



The smallest nut graphs (aka. Sciriha graphs)

Most authors require that a nut graph has $n \geq 2$ vertices.

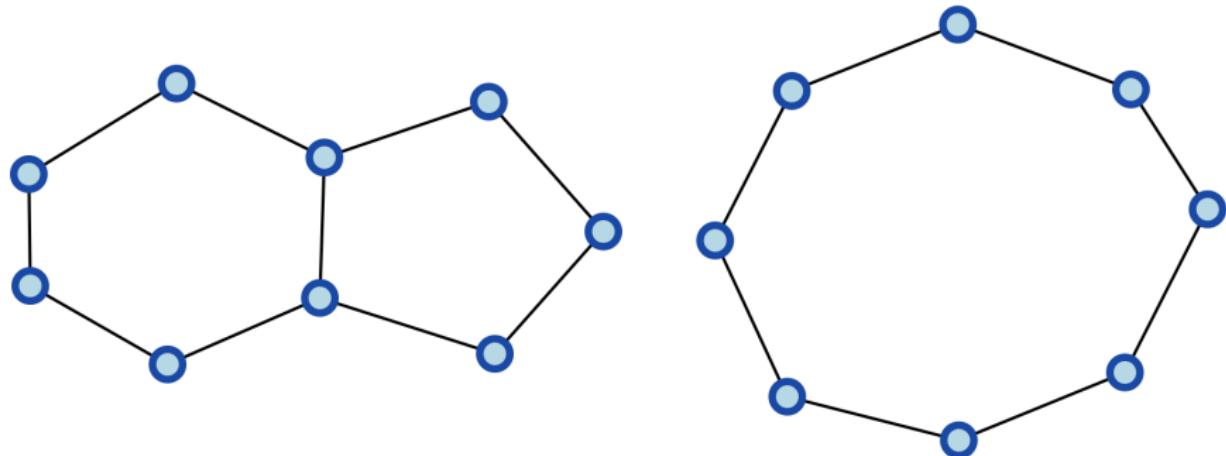
K_1 could, in principle, be considered as the ‘trivial’ nut graph.
It is known that a nut graph must have at least 7 vertices.



Pencil-and-paper method

Application of the local condition

Bad examples:



Some properties of nut graphs

Some simple properties of nut graphs:

- ① Every nut graph is **connected**.
- ② Every nut graphs is **non-bipartite**.
- ③ Every nut graph is **leafless** (i.e. it have no vertices of degree one).

Number of nut graphs

Order	Nut graphs	Connected graphs	% of nuts
0 – 6	0	143	0.0000
7	3	853	0.0035
8	13	11117	0.0012
9	560	261080	0.0021
10	12551	11716571	0.0011
11	2060490	1006700565	0.0020
12	208147869	164059830476	0.0013
13	96477266994	50335907869219	0.0019

See <https://houseofgraphs.org/meta-directory/nut> for more.

Nut graph can be found in the following graph classes: [chemical graphs](#), [cubic graphs](#), [regular graphs](#), [planar graphs](#), [cubic polyhedra](#) (planar 3-connected), [fullerenes](#), ...

Constructions

Obtaining bigger nuts from smaller nuts

A few such constructions:

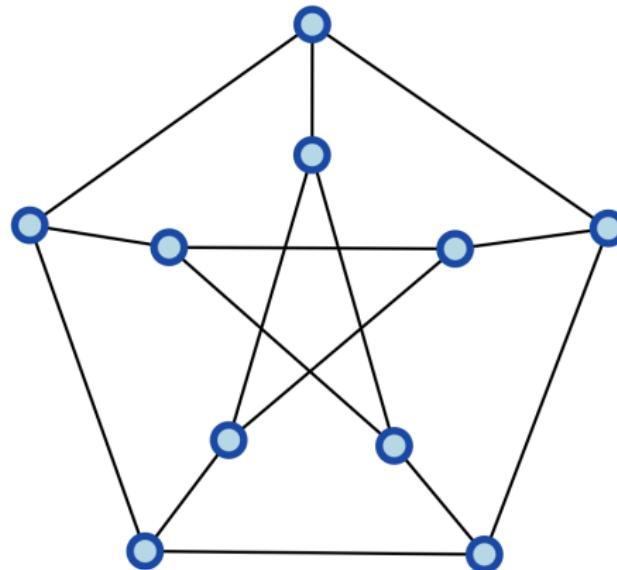
- ① the bridge construction
- ② the subdivision construction
- ③ the Fowler construction

Example (smallest chemical nut graph):

Symmetry

Informally speaking

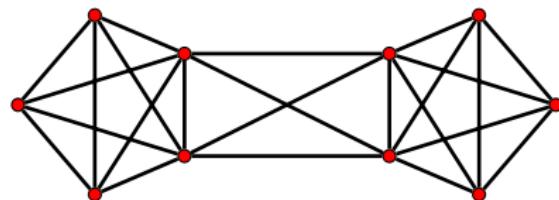
Can we rearrange the vertices somehow and still keep the same graph?



Symmetry

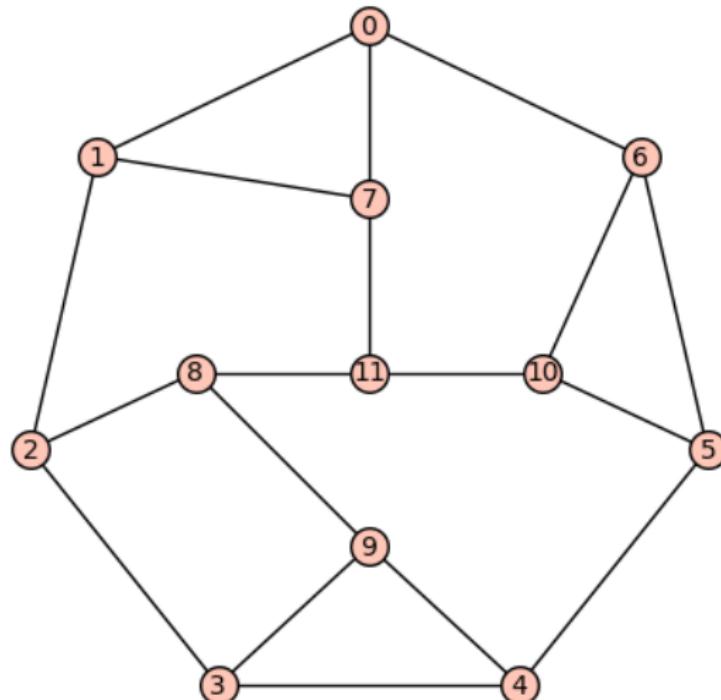
Full automorphism groups of nut graphs on 10 vertices

$ \text{Aut}(G) $	# graphs
1	8951
2	3101
4	394
6	9
8	58
10	1
12	19
16	5
20	1
24	3
32	3
36	2
48	2
72	1
288	1



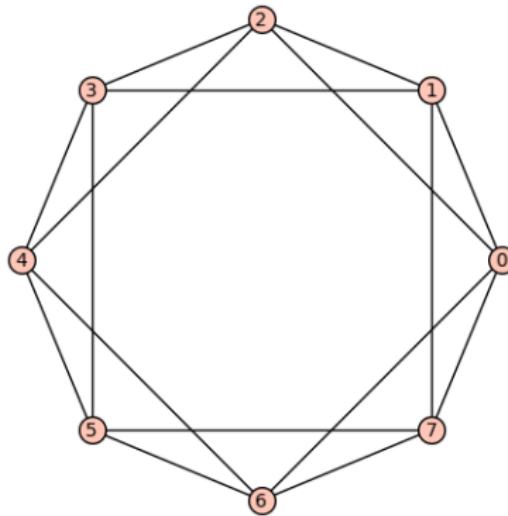
Frucht graph

One of the five smallest cubic asymmetric graphs



Vertex transitive nut graphs exist!

Vertex transitive (VT) nut graphs are graphs with precisely one vertex orbit (v.r.t. the full automorphism group).



$\text{Circ}(8, \{1, 2\})$

What about edge-transitive nut graphs?

Edge transitive (ET) nut graphs are graphs with precisely one edge orbit (v.r.t. the full automorphism group).

Census of ET graphs on orders $n \leq 47$ (by Conder and Verret).

- The census contains 1894 graphs in total. Of these, 335 graphs are non-singular and 2 graphs have nullity 1 (these graphs are K_1 and P_3).
- There are 1312 core graphs in the census (not counting K_1 as a core).
- Amongst these core graphs, there are 1098 bipartite graphs (945 non-regular graphs, 25 regular non-VT graphs and 128 VT graphs).
- The remaining 214 non-bipartite edge-transitive core graphs are necessarily VT, but none of these are nut graphs :^)

If they exist, what do they look like?

Lemma (Folklore)

Let G be an edge-transitive graph with no isolated vertices. If G is not vertex transitive, then $\text{Aut}(G)$ has exactly two orbits, and these two orbits are a bipartition of G .

The above lemma immediately implies:

Corollary

If H is an edge-transitive nut graph, then H is vertex transitive.

If they exist, what do they look like?

Theorem

Let G be a vertex-transitive nut graph on n vertices, of degree d . Then n and d satisfy the following conditions. Either

- $d \equiv 0 \pmod{4}$, and $n \equiv 0 \pmod{2}$ and $n \geq d + 4$; or
- $d \equiv 2 \pmod{4}$, and $n \equiv 0 \pmod{4}$ and $n \geq d + 6$.

It follows immediately that:

Corollary

If H is an edge-transitive nut graph, then H is vertex-transitive and of even degree and even order.

What else can we say about their structure?

Lemma

Let G be a vertex-transitive nut graph and let

$\mathbf{x} = [x_1 \dots x_n]^\top \in \ker A(G)$. Then the following statements hold:

- ① $\mathbf{x} = \pm \mathbf{x}^\alpha$ for every $\alpha \in \text{Aut}(G)$;
- ② $|x_i| = |x_j|$ for all i and j ;
- ③ we can take the entries to be $x_i \in \{+1, -1\}$.

The main result

Theorem

Let G be a nut graph. Then G is not edge transitive.

Proof idea:

Constructions & symmetry

Example: smallest chemical nut graph + bridge construction

Enumeration

Vertex-transitive nut graphs

$n \backslash o_e$	8	10	12	14	16	18	20	22	24	26	28	30	32
1	0	0	0	0	0	0	0	0	0	0	0	0	0
2	1	1	2	2	3	4	6	4	6	8	8	7	1
3	—	—	0	0	3	1	3	0	12	7	7	11	0
4	—	—	0	2	1	7	9	18	51	36	31	73	0
5	—	—	2	0	5	1	20	0	93	0	79	47	7
6	—	—	—	1	6	6	32	38	164	119	277	258	18
7	—	—	—	—	2	0	30	0	181	0	306	98	30
8	—	—	—	—	—	0	21	4	131	34	312	171	45
9	—	—	—	—	—	4	16	32	222	186	756	1078	88
10	—	—	—	—	—	—	9	0	97	5	505	70	282
11	—	—	—	—	—	—	3	0	100	0	924	23	204
12	—	—	—	—	—	—	1	5	41	105	755	1013	173
13	—	—	—	—	—	—	—	—	20	0	476	1	399
14	—	—	—	—	—	—	—	—	3	0	197	0	787
15	—	—	—	—	—	—	—	—	—	8	110	284	2207
16	—	—	—	—	—	—	—	—	—	—	39	0	1110
17	—	—	—	—	—	—	—	—	—	—	9	0	682
18	—	—	—	—	—	—	—	—	—	—	2	12	241
19	—	—	—	—	—	—	—	—	—	—	—	—	52
20	—	—	—	—	—	—	—	—	—	—	—	—	2

PWF and the Goldhorn



Enumeration

Nut graphs with precisely two vertex orbits

$o_e \backslash n$	9	10	12	14	15	16	18	20	21	22	24	25	26	27
1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	1	1	4	7	6	7	10	20	10	19	33	13	26	19
4	—	3	6	2	16	12	16	72	62	6	169	46	19	124
5	—	—	12	1	5	24	78	133	40	20	665	66	44	90
6	—	—	6	3	6	31	99	134	48	122	1460	160	327	227
7	—	—	5	1	3	31	133	171	77	94	3418	191	348	445
8	—	—	4	1	0	78	102	310	77	110	7031	234	552	671
9	—	—	1	—	0	53	136	264	40	184	12081	429	1118	777
10	—	—	—	—	1	80	71	381	88	45	19694	599	283	1984
11	—	—	—	—	—	73	82	392	193	14	28013	156	340	5192
12	—	—	—	—	—	49	18	366	4	154	36902	574	2258	797
13	—	—	—	—	—	17	20	165	49	0	41123	267	77	3996
14	—	—	—	—	—	13	2	147	—	0	44395	8	4	292
15	—	—	—	—	—	3	—	238	—	0	39101	1	15	261
16	—	—	—	—	—	—	—	52	—	10	36325	0	735	420
17	—	—	—	—	—	—	—	9	—	—	24477	0	0	1239
18	—	—	—	—	—	—	—	18	—	—	19068	2	0	136
19	—	—	—	—	—	—	—	1	—	—	8568	2	0	171
20	—	—	—	—	—	—	—	—	—	—	5638	—	20	—
21	—	—	—	—	—	—	—	—	—	—	2173	—	—	—
22	—	—	—	—	—	—	—	—	—	—	838	—	—	—
23	—	—	—	—	—	—	—	—	—	—	140	—	—	—
24	—	—	—	—	—	—	—	—	—	—	63	—	—	—
25	—	—	—	—	—	—	—	—	—	—	7	—	—	—

Generalisation

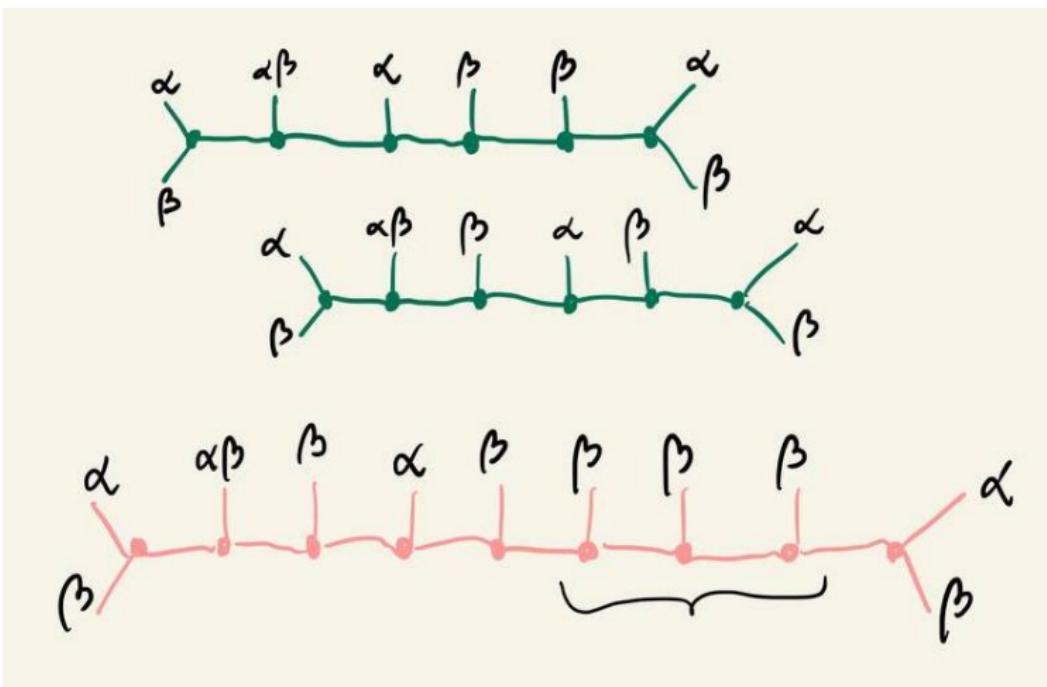
Theorem

Let G be a nut graph. Then $o_e(G) \geq o_v(G) + 1$.

The recent development

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1																						
2																						
3			3																			
4		c1	3																			
5				2	10																	
6		c2	26	5																		
7		c1	5	14	20																	
8		g1+	1	49	12																	
9			8	24	31	47																
10			8	14	48	151	12															
11				4	60	177	60	78														
12		c25	12	70	176	289	56															
13		c140	31	300	400	155	63															
14		g1+	8	136	396	490	450	38														
15		X	p12	107	656	798	999	450	76													
16		p32	35	167	1037	1290	1405	633	68													
17		CL	g4+	26	1282	1683	1982	2035	532	45												
18		g3+	c12	587	686	1325	3019	2762	533	19												
19		g2+	CL	33	120	567	2035	4382	2755	463	8											
20		g1+	CL	3	71	489	2668	6026	3993	201												
21		CL	CL	c2264	c5034	58	874	5215	10262	2183	167											
22		CL	c203	c503	1	99	2303	11745	9775	3179	13											
23		CL	g4+	c13	c141	5	633	7207	20020	17859	575											
24		g3+	CL	c6	c63	24	5388	21839	49864	6964	587											
25		g2+	CL	CL	p898	1	710	8708	68134	31262	7216	3										
26		g1+	CL	c5	9	1089	41589	97465	52073	2073	177											
27		CL	CL	p150	p679	c69	3833	20741	120505	190554	4880											
28		CL	p16	p101	c1	c222	1012	31016	535844	39080												
29		CL	g4+	p5	p50	c3	c1069	16978	377187	83387												
30		g3+	CL	p2	p1	p3	3	167989	345433													
31		g2+	CL	CL	CL	p1	c615	5398	331738													
32		g1+	CL	CL	CL	CL	c5280	22762														
33		CL	CL	CL	CL	CL	I4	7														
34		CL	CL	CL	CL	CL	f1															
35		CL	g4+	CL	CL	CL	CL	f1														
36		g2+	CL	CL	CL	CL	CL	f1														
37																						

The recent development



Long story short:

ET might want to phone home, but he is not a nut.



Thank you!