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More Trees with Large Energy and Small Size

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Abstract

In a previous paper [E. O. D. Andriantiana, *MATCH Commun. Math Comput. Chem.* **68** (2012) 000–000] trees with a fixed number n of vertices were ordered according to their energy, and a large number of trees with greatest energy were characterized. These results, however, hold only if n is large enough. We now analyze the energy–ordering of trees for small values of n (up to 100) and establish the first few greatest–energy species. The results obtained for small values of n significantly differ from those valid for large values of n.

1. Introduction

The search for trees having the greatest value of energy started in 1977 when one of the present authors demonstrated [1] that among n-vertex trees, the path P_n has maximal energy. In the same work [1] also the second–maximal tree was determined. Eventually, the trees with third–maximal [2] and fourth–maximal energy [3–6] were found. In the preceding paper [7], one of the present authors made a significant break–through and determined a very long sequence of n-vertex greatest–energy trees. However, the applicability of the results of [7] is restricted to "large enough n". This "large enough" is over 20000 for odd and over 30000 for even n. The obvious question is what can be said if n assumes values that usually are encountered in chemical graph theory, where the condition $n \leq 100$ is almost always satisfied. The present note is aimed at providing an answer to this question.

The present note should be considered as a continuation of the preceding article [7], and our notation and terminology follows that of [7]. In addition, the ordering of trees specified in Theorem 5 of [7] will be referred here as the $\mathcal{A}$-ordering.

2. Numerical work

The $\mathcal{A}$-ordering of the n-vertex trees ends with the quadripod $H(2,2,2,2,n)$. Because $H(2,2,2,2,n)$ must possess at least 10 vertices, our numerical studies started at $n = 10$ and went up to (from a practical point of view sufficiently large) $n = 100$.

By calculating the energies of all tripods $T(i,j,n-i-j-1)$ as well as the energy of $H(2,2,2,2,n)$ we determined two quantities – $\Lambda(n)$ and $\Omega(n)$, where

- $\Lambda(n)$ is the length (number of elements) of the sequence of n-vertex trees ordered by decreasing energy, starting at the path P_n and ending at $H(2,2,2,2,n)$, whereas
- $\Omega(n)$ is the ordinal number of the last element of the sequence that agrees with the $\mathcal{A}$-ordering.

When checking the $\mathcal{A}$-ordering for small values of n, care must be made with regard to the following difficulty. In the original $\mathcal{A}$-ordering, in which n is assumed to be very large, it is tacitly understood that each tripod $(i,j,n-i-j-1)$ occurs only once [7]. Thus, for instance, the beginning of the ordering reads:

$$\begin{aligned} P_n &> T(2,2,n-5) > T(2,4,n-7) > \cdots > T(2,7,n-10) \\ &> T(4,4,n-9) > T(2,5,n-8) > \cdots \end{aligned}$$

However, if $n = 15$, then $T(2,7,n-10)$ and $T(2,5,n-8)$ are identical, and thus it is impossible to have

$$En(T(2,7,n-10)) > En(T(4,4,n-9)) > En(T(2,5,n-8)) \ .$$

In such cases $\Omega(n)$ is not unambiguously determined, and then we set it's value as small as possible.

For illustrative purposes we reproduce here the details of our calculations for $n = 14$ and $n = 15$. Other numerical results are available from the authors (from B. F.) upon request.

$n = 14$

no.	tree	structure	energy
1	path	P_{14}	not calculated
2	tripod	(2, 2, 9)	17.06702844
3	tripod	(2, 4, 7)	17.05388342
4	tripod	(2, 5, 6)	17.04709989
5	tripod	(2, 3, 8)	17.03843762
6	tripod	(4, 4, 5)	17.03356721
7	tripod	(3, 4, 6)	17.01756784
8	tripod	(1, 2, 10)	17.01176004
9	quadripod	$H(2,2,2,2,14)$	17.00079126
	tripod	(1, 4, 8)	16.98079923
	tripod	(1, 6, 6)	16.97314685
	tripod	(3, 5, 5)	16.65680380
	...		

Because the quadripod $H(2,2,2,2,14)$ has the 9-th maximal energy, $\Lambda(14) = 9$. According to the $\mathcal{A}$-ordering, it should be $En(2,2,9) > En(2,4,7) > En(4,4,5) > En(2,5,6)$ whereas in reality it is $En(2,2,9) > En(2,4,7) > En(2,5,6) > En(2,3,8)$. Therefore, $\Omega(14) = 3$.

$n = 15$

no.	tree	structure	energy
1	path	P_{15}	not calculated
2	tripod	(2, 2, 10)	18.24079093
3	tripod	(2, 4, 8)	18.22976302
4	tripod	(2, 6, 6)	18.22747910
5	tripod	(4, 4, 6)	18.21625035
6	tripod	(2, 5, 7)	18.20030466
7	tripod	(2, 3, 9)	18.19466631
8	quadripod	$H(2,2,2,2,15)$	18.17508403
	tripod	(1, 2, 11)	18.16937381
	tripod	(4, 5, 5)	18.15608137
	tripod	(3, 4, 7)	18.15012078
	...		

Because the quadripod $H(2,2,2,2,15)$ has the 8-th maximal energy, $\Lambda(15) = 8$. According to the $\mathcal{A}$-ordering, it should be $En(2,4,8) > En(2,6,6) > En(2,5,7) > En(4,4,6)$ whereas in reality it is $En(2,4,8) > En(2,6,6) > En(4,4,6) > En(2,5,7)$. Therefore, $\Omega(15) = 4$.

The results of our calculations for $10 \leq n \leq 100$ are found in Table 1.

n	$\Lambda(n)$	$\Omega(n)$	n	$\Lambda(n)$	$\Omega(n)$	n	$\Lambda(n)$	$\Omega(n)$	n	$\Lambda(n)$	$\Omega(n)$
10	5	3	33	36	16	56	107	24	79	173	66
11	5	3	34	48	13	57	106	40	80	179	36
12	7	3	35	42	22	58	112	25	81	177	68
13	7	3	36	51	14	59	113	41	82	186	37
14	9	3	37	47	24	60	119	26	83	183	70
15	8	4	38	56	15	61	121	43	84	191	38
16	12	4	39	52	26	62	126	27	85	188	72
17	10	4	40	61	16	63	128	46	86	197	39
18	14	5	41	57	28	64	132	28	87	194	74
19	12	5	42	68	17	65	135	49	88	202	40
20	17	6	43	62	29	66	138	29	89	198	76
21	15	5	44	72	18	67	143	52	90	207	41
22	21	7	45	67	29	68	142	30	91	206	78
23	20	6	46	78	19	69	148	55	92	213	42
24	25	8	47	72	30	70	149	31	93	213	81
25	23	6	48	85	20	71	154	57	94	219	43
26	28	9	49	78	31	72	155	32	95	220	83
27	26	9	50	90	21	73	158	59	96	225	112
28	33	10	51	83	32	74	161	33	97	226	85
29	29	10	52	97	22	75	163	61	98	231	115
30	37	11	53	90	33	76	167	34	99	230	87
31	33	15	54	102	23	77	169	64	100	236	118
32	42	12	55	99	34	78	172	35			

Table 1. The number $\Lambda(n)$ of maximal–energy n-vertex trees determined in this work, and the number $\Omega(n)$ of such trees determined by the $\mathcal{A}$-ordering from the paper [7]; for details see text.

3. Discussion and concluding remarks

According to the above definition, $\Lambda(n)$ is the number of maximal–energy n-vertex trees whose structure is determined by us. The first among these is the path P_n, the last is the quadripod $H(2,2,2,2,n)$, whereas all trees in between are tripods. Further, the tree with $\Lambda(n+1)$-th-maximal energy may be either a tripod or a quadripod, and in the present work (as well as in [7]), this has not been decided.

The parameter $\Omega(n)$ indicates how far the maximal–energy trees are determined by the $\mathcal{A}$-ordering, i. e., how far one could apply the results of the work [7].

The data from Table 1 show that the value of $\Lambda(n)$ is much smaller than n. Thus, in the case of trees with small number of vertices, the results of the work [7] can be applied only to a limited extent. Yet, $\Lambda(n)$ is always greater than 4, and except for $n < 14$, much greater than 4. This means that by the method elaborated in [7], one can extend the energy–ordering of trees far beyond what was known until now [1–6].

Because in all examined cases, $\Omega(n)$ is significantly smaller than $\Lambda(n)$, we conclude that in the case of trees with small number of vertices, the $\mathcal{A}$-ordering can be applied only to a limited extent, and its application (if at all) should be done with due caution.

As one could expect, both $\Lambda(n)$ and $\Omega(n)$ increase with n, confirming that the results of the work [7] gain in relevance as the size of the underlying trees increases. The n-dependency of $\Lambda(n)$ and $\Omega(n)$ is shown in Figs. 1 and 2, from which the difference of their behavior for even and odd values of n can be envisaged.

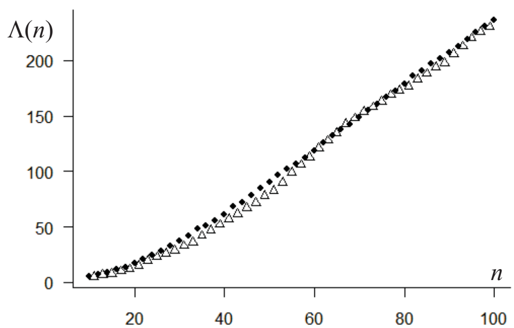

Fig. 1. Dependence of the parameter Λ on the number n of vertices; full circles and triangles pertain, respectively, to even and odd values of n.

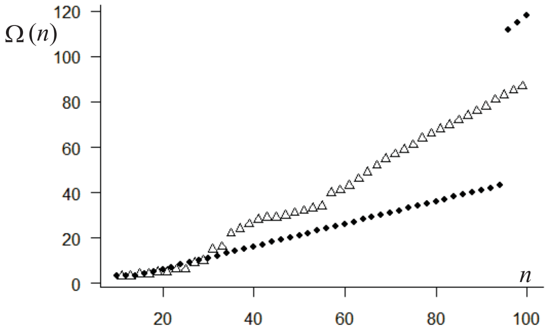

Fig. 2. Dependence of the parameter Ω on the number n of vertices; full circles and triangles pertain, respectively, to even and odd values of n. Note that for even n in the interval $[14, 94]$ the dependence is strictly linear, such that $\Omega(n+2) = \Omega(n) + 1$.

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