

Information entropy of regular dendrimer aggregates and irregular intermediate states

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S U P P L E M E N T A R Y M A T E R I A L S

Section A. Derivation of equations (5)–(7).

First, we extract term $\log_2 N$ from equation (3). Taking into account that

$$\log_2 \frac{ba^{i-1}}{N} = \log_2 ba^{i-1} + \log_2 \frac{1}{N},$$

we rewrite equation (2) as

$$h = -\frac{1}{N} \log_2 \frac{1}{N} - \sum_{i=1}^n \frac{ba^{i-1}}{N} \log_2 ba^{i-1} - \sum_{i=1}^n \frac{ba^{i-1}}{N} \log_2 \frac{1}{N}.$$

Uniting similar terms in the latter expression, we obtain:

$$h = \log_2 N - \sum_{i=1}^n \frac{ba^{i-1}}{N} \log_2 ba^{i-1}.$$

Further, we consider only the second term containing summation. It is simplified as:

$$\begin{aligned} \sum_{i=1}^n \frac{ba^{i-1}}{N} \log_2 ba^{i-1} &= \sum_{i=1}^n \frac{ba^{i-1}}{N} \log_2 b + \sum_{i=1}^n \frac{ba^{i-1}}{N} \log_2 a^{i-1} \\ &= \frac{N-1}{N} \log_2 b + \frac{b}{N} \log_2 a \times \sum_{i=1}^n i a^{i-1} - \frac{b}{N} \log_2 a \times \sum_{i=1}^n a^{i-1} \end{aligned}$$

Designate for clarity the partial sums in the second and third terms as A_1 and A_2 and simplify them separately:

$$\begin{aligned} A_1 &= \frac{b}{N} \log_2 a \times \sum_{i=1}^n i a^{i-1} = \frac{b}{N} \left(\frac{na^{n+1} - (n+1)a^{n+1}}{(a-1)^2} \right) \log_2 a, \\ A_2 &= -\frac{b}{N} \log_2 a \times \sum_{i=1}^n a^{i-1} = -\frac{N-1}{N} \log_2 a. \end{aligned}$$

Hence:

$$-h_{fract} = \frac{N-1}{N} \log_2 b + A_1 + A_2 = \frac{N-1}{N} \log_2 b + \frac{b}{N} \frac{na^{n+1} - (n+1)a^{n+1}}{(a-1)^2} \log_2 a - \frac{N-1}{N} \log_2 a$$

or

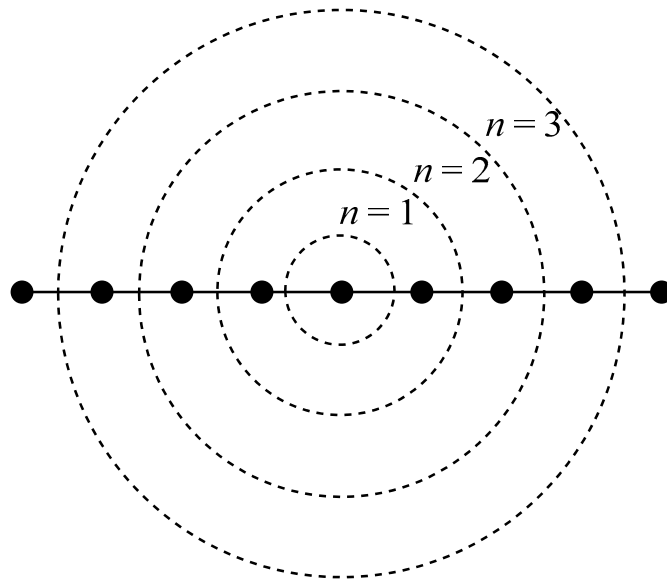
$$h_{fract} = \frac{N-1}{N} \log_2 \frac{a}{b} - \frac{b}{N} \frac{na^{n+1} - (n+1)a^{n+1}}{(a-1)^2} \log_2 a$$

Section B. Information entropy of linear polymer deduced from equation (2).

Considering coordination number b equal to 2, we have the linear polymer with odd number of building blocks $N = 2n + 1$. The structure is presented in **Figure** below. Its partition is $1 \times 1 + n \times 2$. Then using equation (2), we obtain:

$$\begin{aligned} h &= -\frac{1}{2n+1} \log_2 \frac{1}{2n+1} \\ &\quad - \frac{2n}{2n+1} \log_2 \frac{2}{2n+1} \\ &= \frac{1}{2n+1} \log_2(2n+1) - \frac{2n}{2n+1} \log_2 2 + \frac{2n}{2n+1} \log_2(2n+1) = \log_2(2n+1) - \frac{2n}{2n+1} \end{aligned}$$

The same result is obtained from equations (5)–(7).



Section C. Numerical data associated with Figure 2. The h values are in bits.*

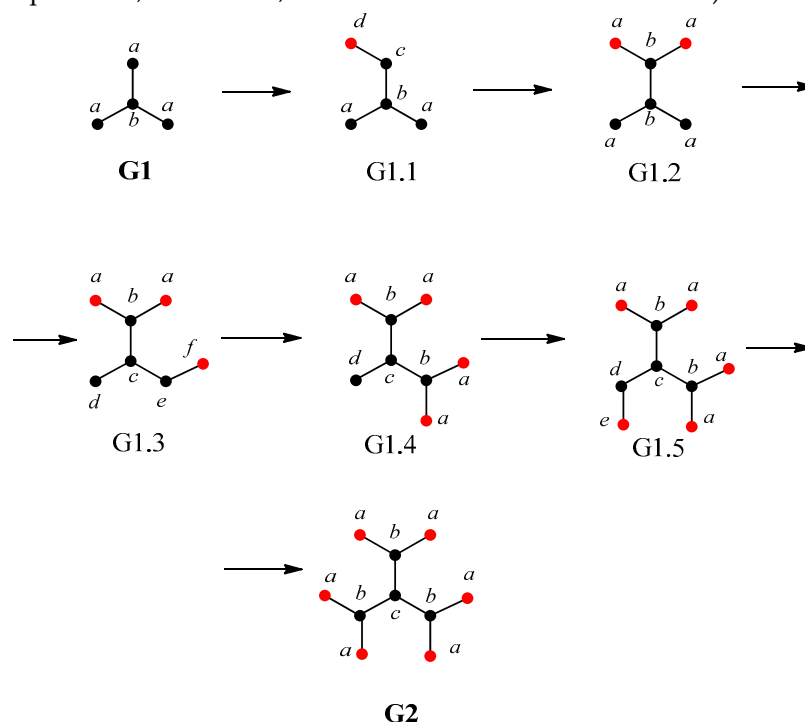
Number of generation (n)	Coordination of the building block			
	$b = 3$	$b = 4$	$b = 5$	$b = 6$
1	0.8112781245	0.7219280949	0.6500224216	0.5916727786
2	1.2954618442	1.0863128407	0.9293550115	0.8117103150
3	1.5828765043	1.2536402647	1.0316709266	0.8782351206
4	1.7556638575	1.3267883049	1.0661193847	0.8963455947
5	1.8588280797	1.3573541304	1.0770306524	0.9009499998
6	1.9195508050	1.3696678973	1.0803407777	0.9020685829
7	1.9547306271	1.3744904670	1.0813145132	0.9023319057
8	1.9748085283	1.3763386689	1.0815945474	0.9023924947
9	1.9861156791	1.3770351449	1.0816737097	0.9024061976
10	1.9924105902	1.3772941304	1.0816957889	0.9024092551
11	1.9958808274	1.3773894042	1.0817018810	0.9024099301
12	1.9977779430	1.3774241443	1.0817035470	0.9024100777
13	1.9988076703	1.3774367184	1.0817039993	0.9024101098
14	1.9993631665	1.3774412412	1.0817041213	0.9024101167
15	1.9996612439	1.3774428592	1.0817041540	0.9024101182
16	1.9998204510	1.3774434354	1.0817041628	0.9024101185
17	1.9999051396	1.3774436397	1.0817041651	0.9024101186
18	1.9999500268	1.3774437119	1.0817041657	0.9024101186
19	1.9999737419	1.3774437373	1.0817041659	0.9024101186
20	1.9999862352	1.3774437463	1.0817041659	0.9024101186

* Obtained *via* equations (5)–(7).

Section D. Transition structures between G1 and G2 according to path I.

Structure code according to Schematic below	Total number of building blocks	Partition ([number of types]×[number of blocks within the type])	Information entropy (bits)
G1 (regular dendrimer)	4	1×3 + 1×1	0.811
G1.1	5	1×2 + 3×1	1.922
G1.2	6	1×4 + 1×2	0.918
G1.3	7	1×2 + 5×1	2.522
G1.4	8	1×4 + 1×2 + 2×1	1.750
G1.5	9	1×4 + 1×2 + 3×1	2.059
G2 (regular dendrimer)	10	1×6 + 1×3 + 1×1	1.295

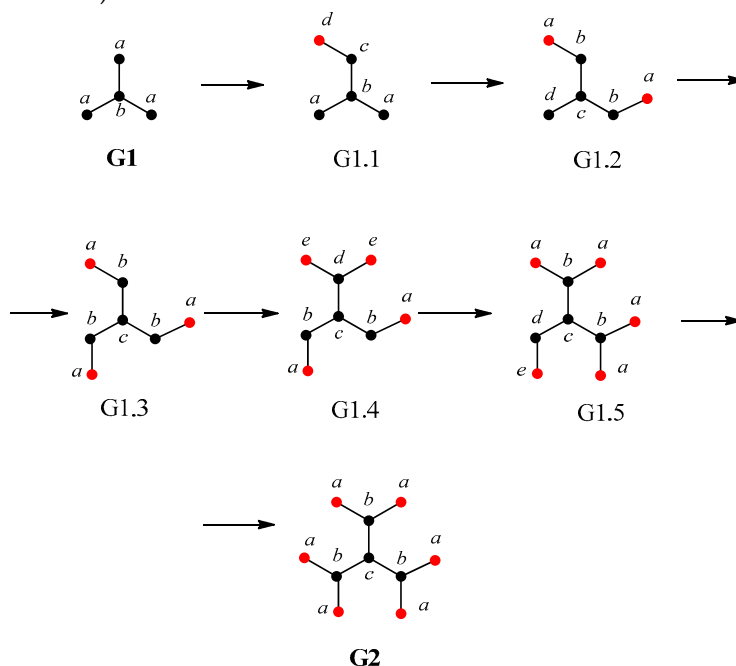
Schematic of transformation G1 → G2 according to path I (the blocks are lettered according to the equivalence of their positions; hereinafter, new added blocks are shown in red)



Section E. Transition structures between G1 and G2 according to path II.

Structure code according to Schematic below	Total number of building blocks	Partition ([number of types]×[number of blocks within the type])	Information entropy (bits)
G1 (regular dendrimer)	4	1×3 + 1×1	0.811
G1.1	5	1×2 + 3×1	1.922
G1.2	6	2×2 + 2×1	1.918
G1.3	7	2×3 + 1×1	1.449
G1.4	8	3×2 + 2×1	2.250
G1.5	9	1×4 + 1×2 + 3×1	2.059
G2 (regular dendrimer)	10	1×6 + 1×3 + 1×1	1.295

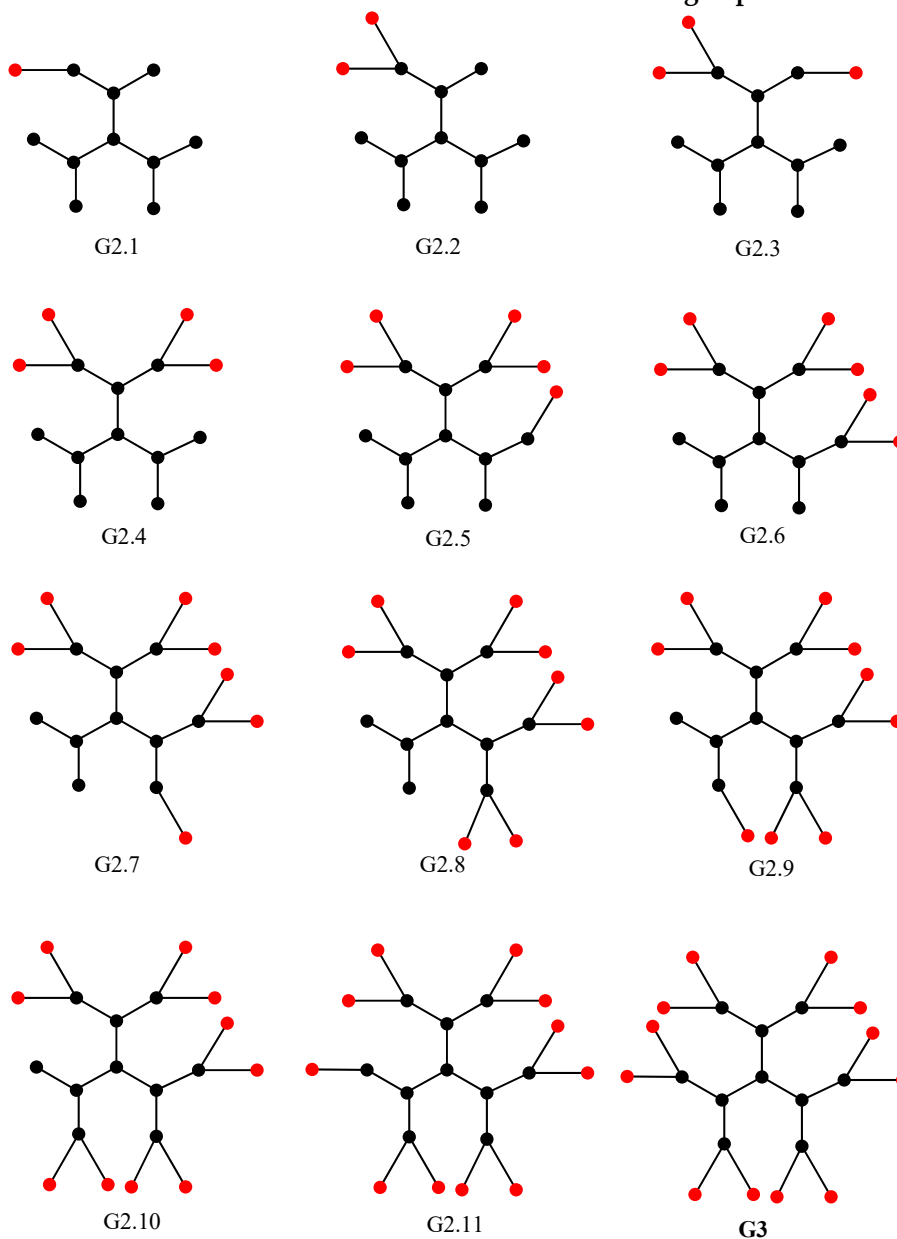
Schematic of transformation G1 → G2 according to path II (the blocks are lettered according to the equivalence of their positions)



Section F. Transition structures between G2 and G3 according to path I.

Structure code according to Schematic below	Total number of building blocks	Partition ([number of types]×[number of blocks within the type])	Information entropy (bits)
G2 (regular dendrimer)	10	1×6 + 1×3 + 1×1	1.295
G2.1	11	1×4 + 1×2 + 5×1	2.550
G2.2	12	1×4 + 2×2 + 4×1	2.585
G2.3	13	1×4 + 2×2 + 5×1	2.777
G2.4	14	1×8 + 1×4 + 1×2	1.379
G2.5	15	1×4 + 2×2 + 7×1	3.107
G2.6	16	1×4 + 3×2 + 6×1	3.125
G2.7	17	1×4 + 3×2 + 7×1	3.264
G2.8	18	1×8 + 1×4 + 2×2 + 2×1	2.170
G2.9	19	1×8 + 1×4 + 1×2 + 5×1	2.458
G2.10	20	1×8 + 1×4 + 2×2 + 4×1	2.522
G2.11	21	1×8 + 1×4 + 2×2 + 5×1	2.678
G3 (regular dendrimer)	22	1×12 + 1×6 + 1×3 + 1×1	1.583

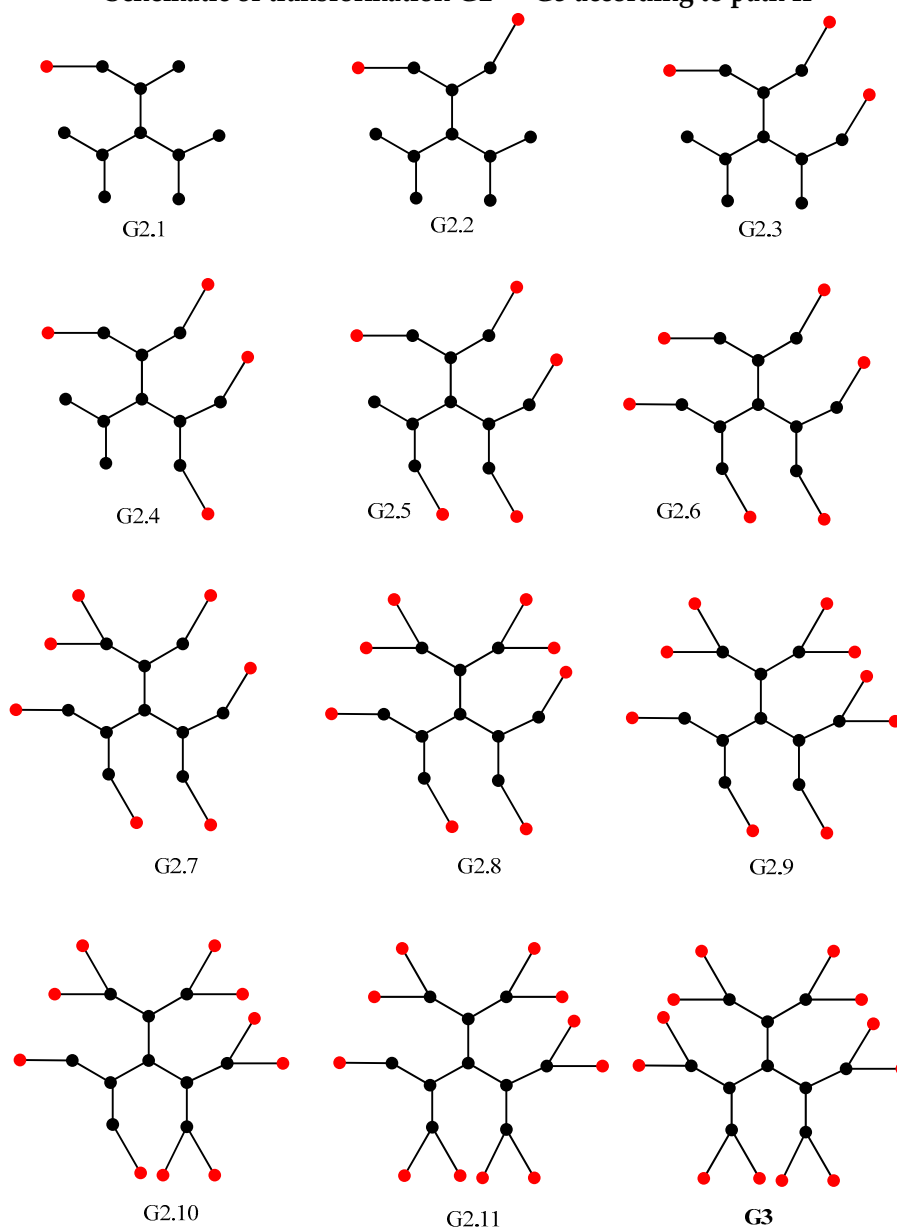
Schematic of transformation G2 → G3 according to path I



Section G. Transition structures between G2 and G3 according to path II.

Structure code according to Schematic below	Total number of building blocks	Partition ([number of types]×[number of blocks within the type])	Information entropy (bits)
G2 (regular dendrimer)	10	1×6 + 1×3 + 1×1	1.295
G2.1	11	1×4 + 1×2 + 5×1	2.550
G2.2	12	1×4 + 3×2 + 2×1	2.418
G2.3	13	3×2 + 7×1	3.239
G2.4	14	2×4 + 2×2 + 2×1	2.379
G2.5	15	2×4 + 1×2 + 5×1	2.707
G2.6	16	2×6 + 1×3 + 1×1	1.764
G2.7	17	2×4 + 2×2 + 5×1	2.911
G2.8	18	3×4 + 2×2 + 2×1	2.614
G2.9	19	1×4 + 4×2 + 7×1	3.406
G2.10	20	1×8 + 1×4 + 3×2 + 2×1	2.422
G2.11	21	1×8 + 1×4 + 2×2 + 5×1	2.678
G3 (regular dendrimer)	22	1×12 + 1×6 + 1×3 + 1×1	1.583

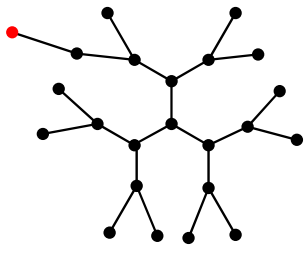
Schematic of transformation G2 → G3 according to path II



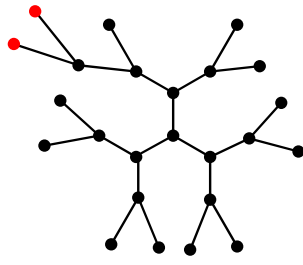
Section H. Transition structures between G3 and G4 according to path I.

Structure code according to Schematic below	Total number of building blocks	Partition ([number of types]×[number of blocks within the type])	Information entropy (bits)
G3 (regular dendrimer)	22	$1 \times 12 + 1 \times 6 + 1 \times 3 + 1 \times 1$	1.583
G3.1	23	$1 \times 8 + 1 \times 4 + 2 \times 2 + 7 \times 1$	2.958
G3.2	24	$1 \times 8 + 1 \times 4 + 3 \times 2 + 6 \times 1$	3.002
G3.3	25	$1 \times 8 + 1 \times 4 + 3 \times 2 + 7 \times 1$	3.124
G3.4	26	$1 \times 8 + 2 \times 4 + 3 \times 2 + 4 \times 1$	2.931
G3.5	27	$1 \times 8 + 2 \times 4 + 2 \times 2 + 7 \times 1$	3.125
G3.6	28	$1 \times 8 + 2 \times 4 + 3 \times 2 + 6 \times 1$	3.164
G3.7	29	$1 \times 8 + 2 \times 4 + 3 \times 2 + 7 \times 1$	3.272
G3.8	30	$1 \times 16 + 1 \times 8 + 1 \times 4 + 1 \times 2$	1.640
G3.9	31	$1 \times 8 + 2 \times 4 + 3 \times 2 + 9 \times 1$	3.470
G3.10	32	$1 \times 8 + 2 \times 4 + 4 \times 2 + 8 \times 1$	3.500
G3.11	33	$1 \times 8 + 2 \times 4 + 4 \times 2 + 9 \times 1$	3.590
G3.12	34	$1 \times 8 + 3 \times 4 + 4 \times 2 + 6 \times 1$	3.440
G3.13	35	$1 \times 8 + 3 \times 4 + 3 \times 2 + 9 \times 1$	3.586
G3.14	36	$1 \times 8 + 3 \times 4 + 4 \times 2 + 8 \times 1$	3.614
G3.15	37	$1 \times 8 + 3 \times 4 + 4 \times 2 + 9 \times 1$	3.696
G3.16	38	$1 \times 16 + 1 \times 8 + 2 \times 4 + 2 \times 2 + 2 \times 1$	2.406
G3.17	39	$1 \times 16 + 1 \times 8 + 1 \times 4 + 2 \times 2 + 7 \times 1$	2.721
G3.18	40	$1 \times 16 + 1 \times 8 + 1 \times 4 + 3 \times 2 + 6 \times 1$	2.772
G3.19	41	$1 \times 16 + 1 \times 8 + 1 \times 4 + 3 \times 2 + 7 \times 1$	2.870
G3.20	42	$1 \times 16 + 1 \times 8 + 2 \times 4 + 3 \times 2 + 4 \times 1$	2.773
G3.21	43	$1 \times 16 + 1 \times 8 + 2 \times 4 + 2 \times 2 + 7 \times 1$	2.915
G3.22	44	$1 \times 16 + 1 \times 8 + 2 \times 4 + 3 \times 2 + 6 \times 1$	2.959
G3.23	45	$1 \times 16 + 1 \times 8 + 2 \times 4 + 3 \times 2 + 7 \times 1$	3.047
G4 (regular dendrimer)	46	$1 \times 24 + 1 \times 12 + 1 \times 6 + 1 \times 3 + 1 \times 1$	1.756

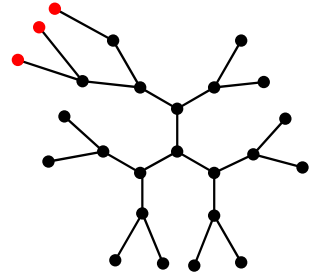
Schematic of transformation $G3 \rightarrow G4$ according to path I



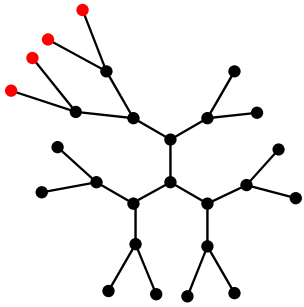
G3.1



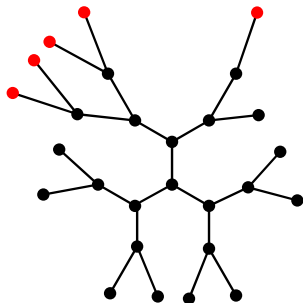
G3.2



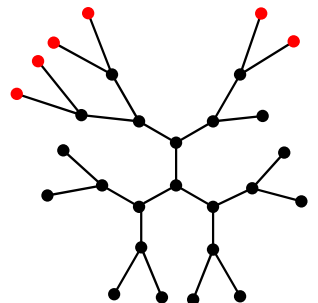
G3.3



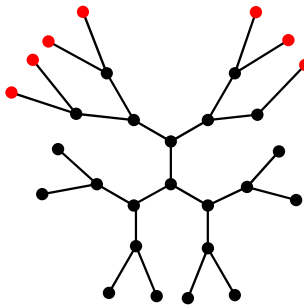
G3.4



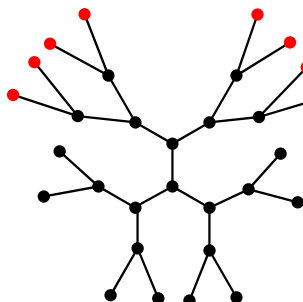
G3.5



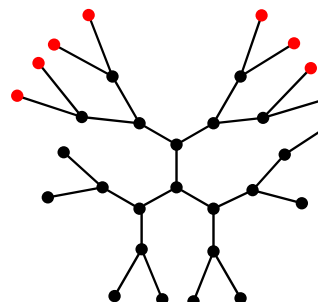
G3.6



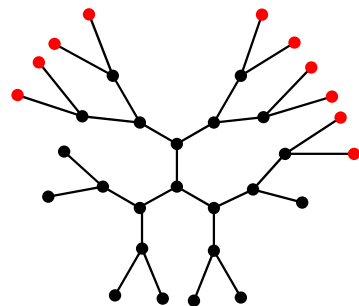
G3.7



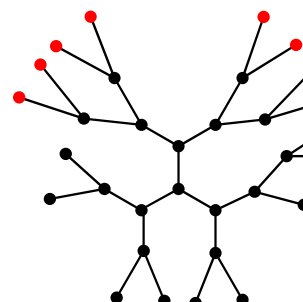
G3.8



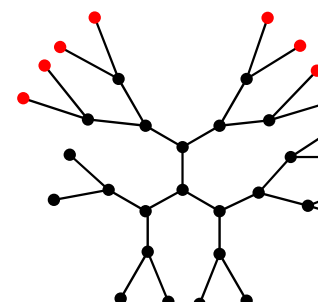
G3.9



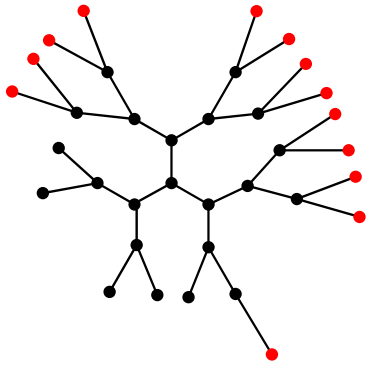
G3.10



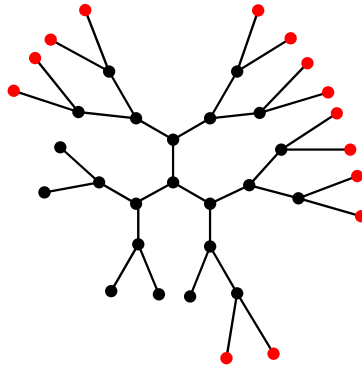
G3.11



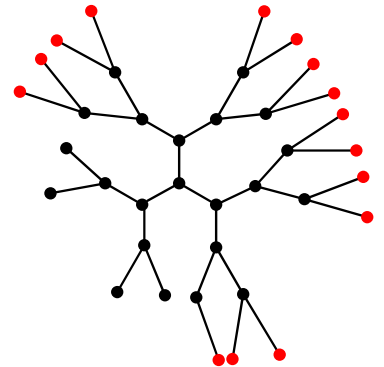
G3.12



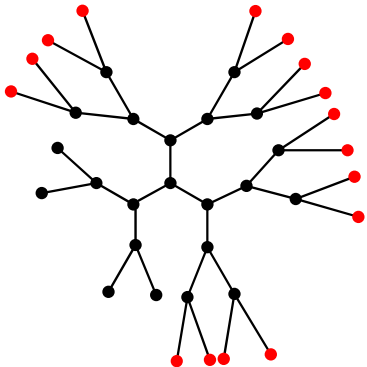
G3.13



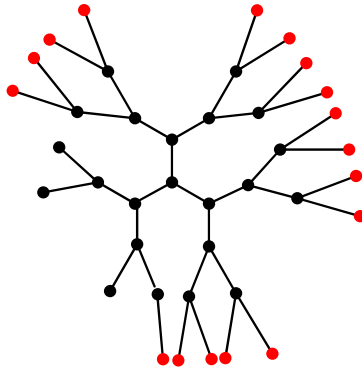
G3.14



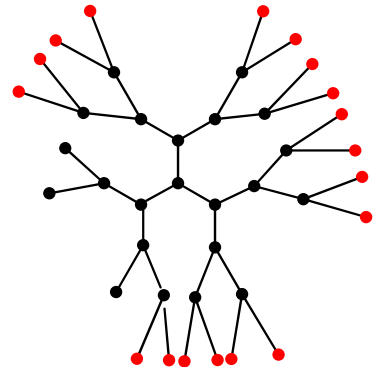
G3.15



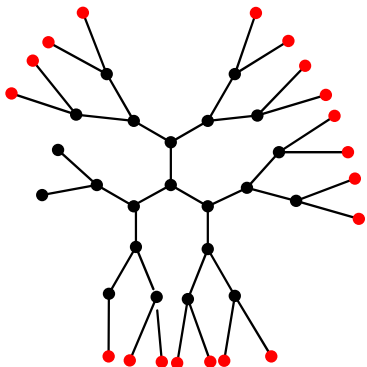
G3.16



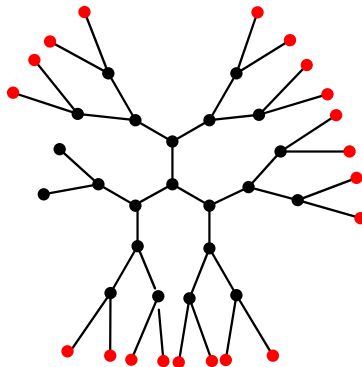
G3.17



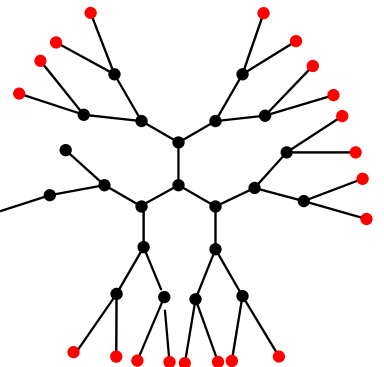
G3.18



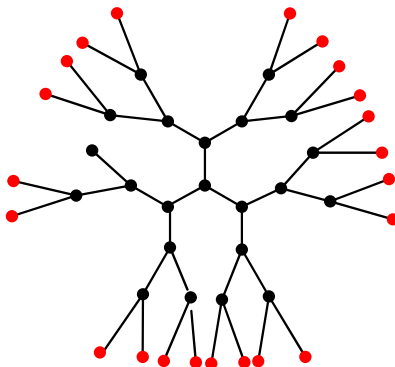
G3.19



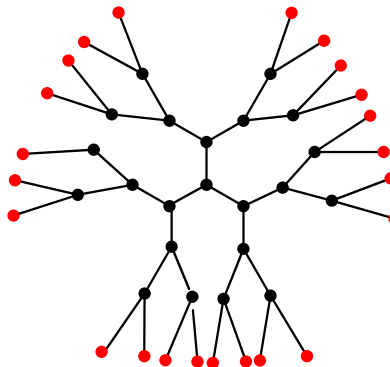
G3.20



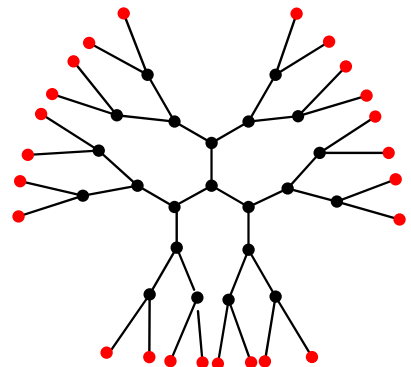
G3.21



G3.22



G3.23

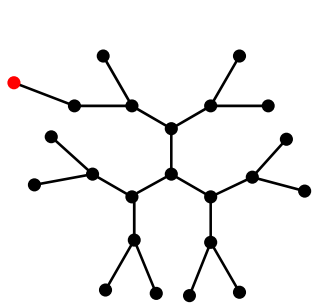


G4

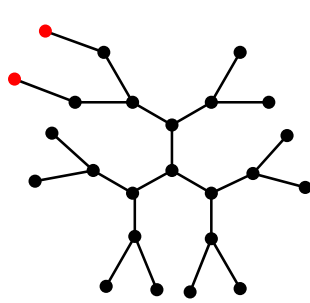
Section I. Transition structures between G3 and G4 according to path II.

Structure code according to Schematic below	Total number of building blocks	Partition ([number of types]×[number of blocks within the type])	Information entropy (bits)
G3 (regular dendrimer)	22	$1 \times 12 + 1 \times 6 + 1 \times 3 + 1 \times 1$	1.583
G3.1	23	$1 \times 8 + 1 \times 4 + 2 \times 2 + 7 \times 1$	2.958
G3.2	24	$1 \times 8 + 1 \times 4 + 4 \times 2 + 4 \times 1$	2.918
G3.3	25	$1 \times 8 + 1 \times 4 + 3 \times 2 + 7 \times 1$	3.124
G3.4	26	$1 \times 8 + 3 \times 4 + 2 \times 2 + 2 \times 1$	2.700
G3.5	27	$3 \times 4 + 3 \times 2 + 9 \times 1$	3.644
G3.6	28	$3 \times 4 + 5 \times 2 + 6 \times 1$	3.593
G3.7	29	$3 \times 4 + 4 \times 2 + 9 \times 1$	3.755
G3.8	30	$2 \times 8 + 2 \times 4 + 3 \times 2 + 2 \times 1$	2.813
G3.9	31	$2 \times 8 + 1 \times 4 + 2 \times 2 + 7 \times 1$	3.019
G3.10	32	$2 \times 8 + 1 \times 4 + 4 \times 2 + 4 \times 1$	3.000
G3.11	33	$2 \times 8 + 1 \times 4 + 3 \times 2 + 7 \times 1$	3.166
G3.12	34	$2 \times 8 + 3 \times 4 + 2 \times 2 + 2 \times 1$	2.852
G3.13	35	$2 \times 8 + 1 \times 4 + 4 \times 2 + 7 \times 1$	3.301
G3.14	36	$2 \times 8 + 2 \times 4 + 4 \times 2 + 4 \times 1$	3.170
G3.15	37	$2 \times 8 + 2 \times 4 + 4 \times 2 + 5 \times 1$	3.264
G3.16	38	$3 \times 8 + 2 \times 4 + 2 \times 2 + 2 \times 1$	2.827
G3.17	39	$1 \times 8 + 3 \times 4 + 5 \times 2 + 9 \times 1$	3.798
G3.18	40	$1 \times 8 + 4 \times 4 + 5 \times 2 + 6 \times 1$	3.672
G3.19	41	$1 \times 8 + 4 \times 4 + 4 \times 2 + 9 \times 1$	3.797
G3.20	42	$1 \times 16 + 1 \times 8 + 3 \times 4 + 2 \times 2 + 2 \times 1$	2.630
G3.21	43	$1 \times 16 + 1 \times 8 + 1 \times 4 + 4 \times 2 + 7 \times 1$	3.008
G3.22	44	$1 \times 16 + 1 \times 8 + 2 \times 4 + 4 \times 2 + 4 \times 1$	2.914
G3.23	45	$1 \times 16 + 1 \times 8 + 2 \times 4 + 3 \times 2 + 7 \times 1$	3.047
G4 (regular dendrimer)	46	$1 \times 24 + 1 \times 12 + 1 \times 6 + 1 \times 3 + 1 \times 1$	1.756

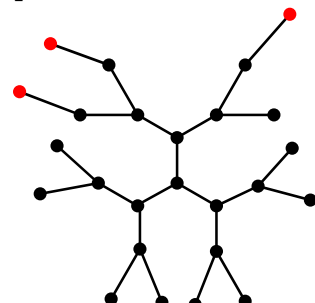
Schematic of transformation $G3 \rightarrow G4$ according to path II



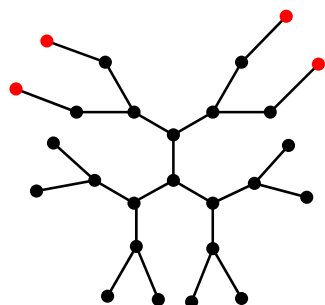
G3.1



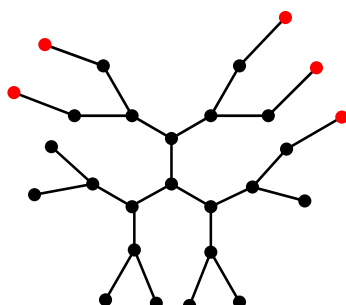
G3.2



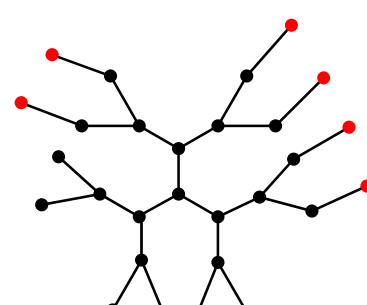
G3.3



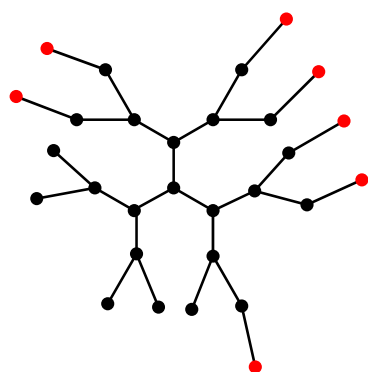
G3.4



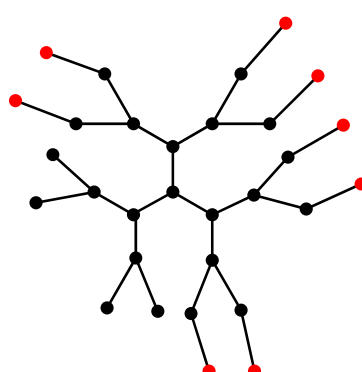
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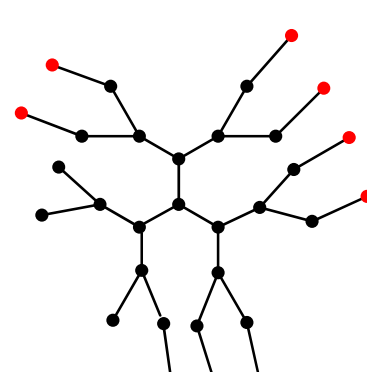
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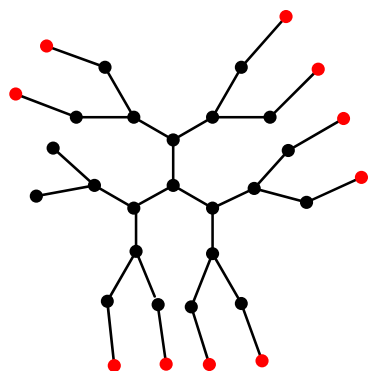
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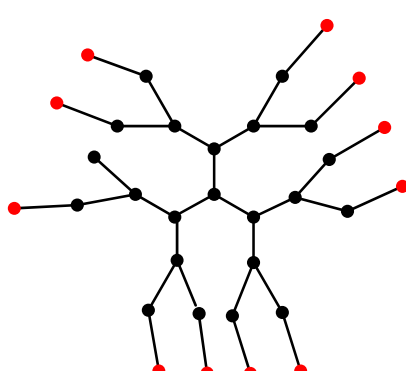
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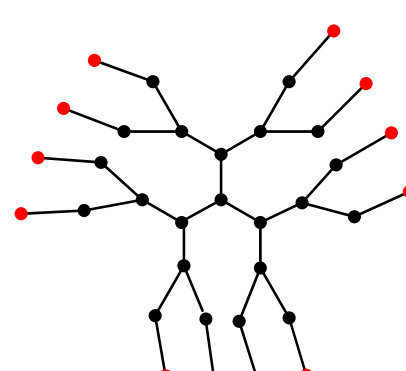
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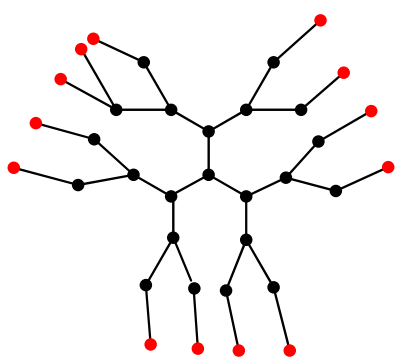
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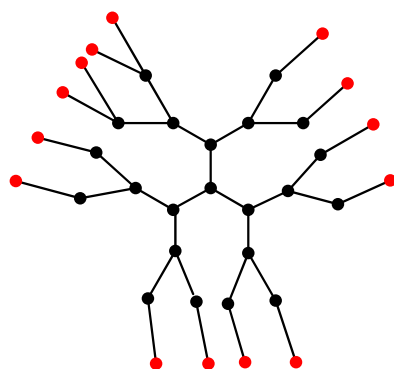
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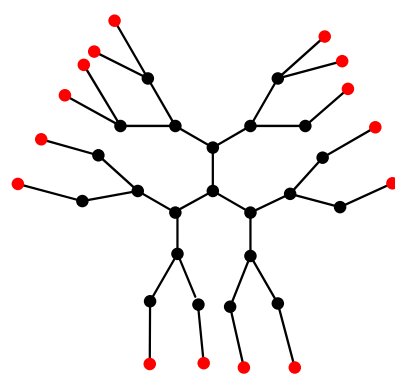
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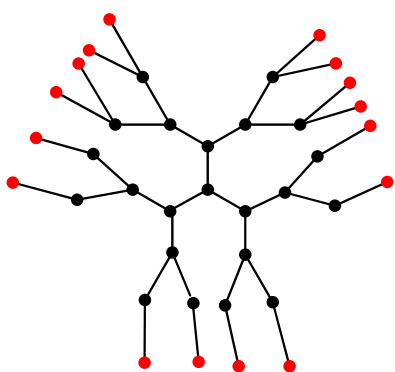
G3.13



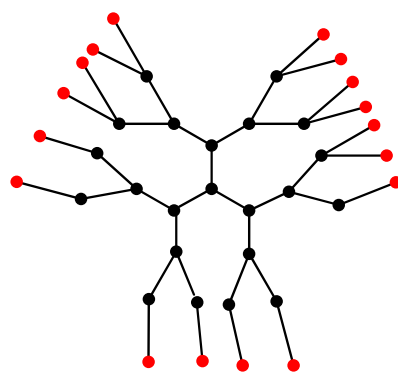
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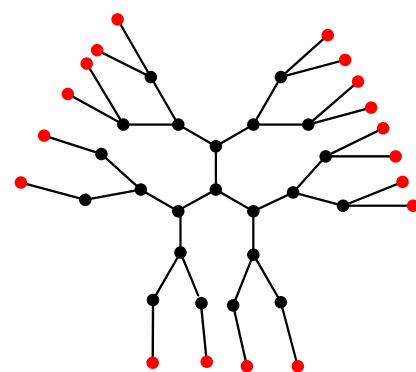
G3.15



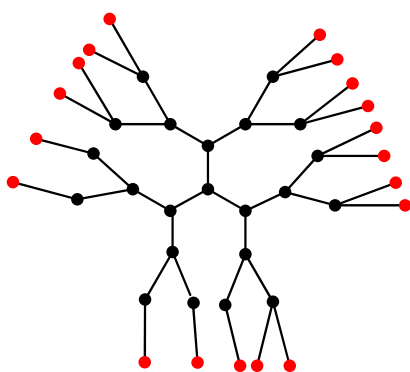
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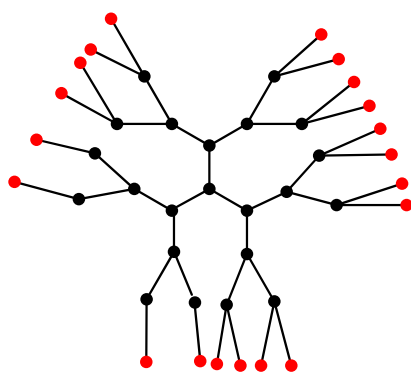
G3.17



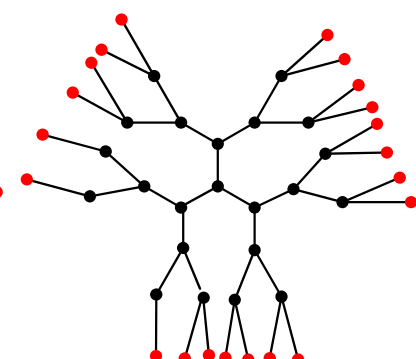
G3.18



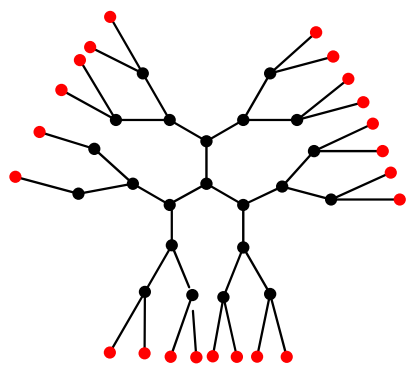
G3.19



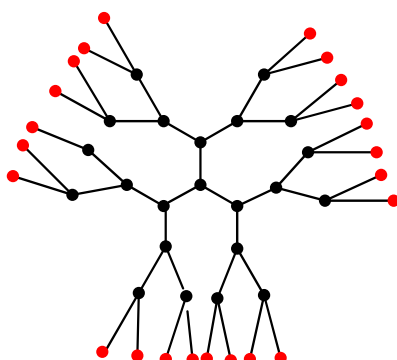
G3.20



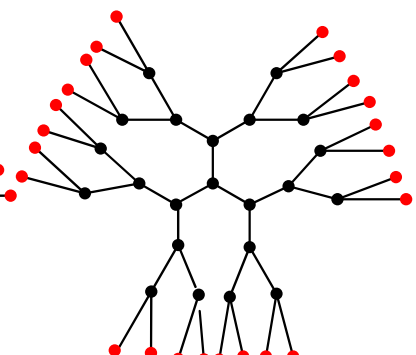
G3.21



G3.22



G3.23



G4