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CLUJ AND RELATED POLYNOMIALS IN TORI

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ABSTRACT. Cluj polynomials are defined on the unsymmetric Cluj matrices or by a cutting procedure, as the counting polynomials which collect the vertex proximities in the graph. On these proximities, two Cluj polynomials CJS and CJP and the PIv polynomial can be defined. Formulas for these counting polynomials are derived in case of tori of several tessellation.

Keywords: *Cluj polynomial, counting polynomial, torus*

INTRODUCTION

Let *G*=*G*(*V*,*E*) be a simple graph, with no loops and multiple edges and V(G), E(G) be its vertex and edge sets, respectively.

A graph *G* is a *partial cube* if it is embeddable in the *n*-cube Q_n, which is the regular graph whose vertices are all binary strings of length *n*, two strings being adjacent if they differ in exactly one position [1]. The distance function in the *n*-cube is the Hamming distance. A hypercube can also be expressed as the Cartesian product: $Q_n = W_{i=1}^{n} K_2$

For any edge *e*=(*u*,*v*) of a connected graph *G* let n_{uv} denote the set of vertices lying closer to *u* than to *v*: $n_{uv} = \{ w \in V(G) \mid d(w,u) < d(w,v) \}$. It follows that $n_{uv} = \{ w \in V(G) \mid d(w,v) = d(w,u) + 1 \}$. The sets (and subgraphs) induced by these vertices, n_{uv} and n_{vu} , are called *semicubes* of *G*; the semicubes are called *opposite semicubes* and are disjoint [2,3].

A graph *G* is bipartite if and only if, for any edge of *G*, the opposite semicubes define a partition of *G*: $n_{uv} + n_{vu} = v = |V(G)|$. These semicubes are just the vertex proximities (see above) of (the endpoints of) edge *e*=(*u*,*v*), which *CJ* polynomial counts. In partial cubes, the semicubes can be estimated by an orthogonal edge-cutting procedure. The orthogonal cuts form a partition of the edges in *G*:

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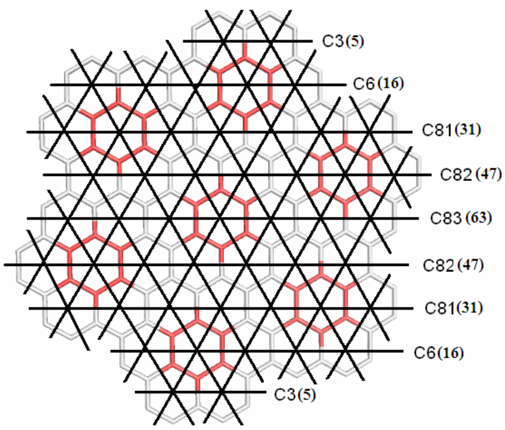
$$E(G) = c_1 \cup c_2 \cup \ldots \cup c_k, c_i \cap c_j = \varnothing, i \neq j .$$

To perform an orthogonal edge-cut, take a straight line segment, orthogonal to the edge *e*, and intersect *e* and all its parallel edges (in a plane graph). The set of these intersections is called an *orthogonal cut* $c_k(e)$ with respect to the edge *e*. An example is given in Table 1.

To any orthogonal cut c_k, two numbers are associated: first one is the *number of edges* $e_k = |c_k|$ intersected by the orthogonal segment while the second (in round brackets, in Figure 1) is v_k or the number of points lying to the left hand with respect to c_k.

Because in bipartite graphs the opposite semicubes define a partition of vertices, it is easily to identify the two semicubes: $n_{uv} = v_k$ and $n_{vu} = v - v_k$ or vice-versa.

The present study is focused on three counting polynomials of which coefficients can be calculated from the graph proximities/semicubes.



$CJS(x)$ = 3·2·3(x^5+x^{121})+ 3·2·6(x^{16}+x^{110})+ 3·2·8(x^{31}+x^{95})+ 3·2·8(x^{47}+x^{79})+ 3·1·8(x^{63}+x^{63})

$CJS'(1)$ = **21924**; $CJ_e\,S''(1)$ = 1762320

$PI_v(x)$ = 3·2·3(x^5+^{121})+ 3·2·6(x^{16}+^{110})+ 3·2·8(x^{31}+^{95})+ 3·2·8(x^{47}+^{79})+ 3·1·8(x^{63}+^{63})

$PI_v'(1)$ = **21924**; $PI_v''(1)$ = 2740500

$CJP(x)$ = 3·2·3($x^{5\cdot 121}$)+ 3·2·6($x^{16\cdot 110}$)+ 3·2·8($x^{31\cdot 95}$)+ 3·2·8($x^{47\cdot 79}$)+3·1·8($x^{63\cdot 63}$)

$CJP'(1)$ = **489090**=$CJP(G)$= $SZ_v'(1)$

Figure 1. Cutting procedure in the calculus of several topological descriptors.

COUNTING POLINOMIALS OF PROXIMITY

According to the mathematical operations used in composing the edge contributions, these polynomials can be defined as [4]:

(i) *Summation*; the polynomial is called *Cluj-Sum* and is symbolized *CJS* -Diudea *et al* [5-9].

$$CJS(x) = \sum_e \left(x^{v_k} + x^{v - v_k} \right) \quad (1)$$

(ii) *Pair-wise summation*; the polynomial is called PI_v (vertex-Padmakar-Ivan [10]) - Ashrafi *et al* [11-14].

$$PI_v(x) = \sum_e x^{v_k + (v - v_k)} \quad (2)$$

(iii) *Pair-wise product*; the polynomial is called *Cluj-Product* (and symbolized *CJP*) [4,8,15-19] or also *Szeged* (and symbolized *SZ*) [12-14]:

$$CJP(x) = SZ(x) = \sum_e x^{v_k(v-v_k)} \tag{3}$$

Their coefficients can be calculated from the graph proximities / semicubes as shown in Figure 1: the product of three numbers (in the front of brackets – right hand of Figure 1) has the meaning: (i) symmetry of *G*; (ii) occurrence of c_k (in the whole structure) and (iii) e_k.

The first derivative (in *x*=1) of a (graph) counting polynomial provides single numbers, often called topological indices.

Observe that the first derivative (in *x*=1) of the first two polynomials gives one and the same value (Figure 1), however, their second derivative is different and the following relations hold in any graph [4,7].

$$CJS'(1) = PI_v'(1);\ CJS''(1) \neq PI_v''(1) \tag{4}$$

The number of terms, given by *P*(1), is: *CJS*(1)=2*e* while $PI_v(1)=e$ because, in the last case, the two endpoint contributions are pair-wise summed for any edge in a bipartite graph.

In bipartite graphs, the first derivative (in *x*=1) of $PI_v(x)$ takes the maximal value:

$$PI_v'(1) = e \cdot v = |E(G)| \cdot |V(G)| \tag{5}$$

It can also be seen by considering the definition of the corresponding index, as written by Ilić [20]:

$$PI_v(G) = PI_v'(1) = \sum_{e=uv} n_{u,v} + n_{v,u} = |V| \cdot |E| - \sum_{e=uv} m_{u,v} \tag{6}$$

where $n_{u,v}$, $n_{v,u}$ count the non-equidistant vertices with respect to the endpoints of the edge *e*=(*u*,*v*) while *m*(*u,v*) is the number of equidistant vertices *vs*. *u* and *v*. However, it is known that, in bipartite graphs, there are no equidistant vertices, so that the last term in (6) will disappear. The value of $PI_v(G)$ is thus maximal in bipartite graphs, among all graphs on the same number of vertices; the result of (5) can be used as a criterion for the “bipatity” of a graph [6].

The third polynomial is calculated as the pair-wise product; notice that Cluj-Product *CJP*(*x*) is precisely the (vertex) Szeged polynomial $SZ_v(x)$, defined by Ashrafi *et al*. [12-14] This comes out from the relations between the basic Cluj (Diudea [16,21,22]) and Szeged (Gutman [22,23]) indices:

$$CJP'(1) = CJDI(G) = SZ(G) = SZ_v'(1) \tag{7}$$

All the three polynomials (and their derived indices) do not count the equidistant vertices, an idea introduced in Chemical Graph Theory by Gutman [23].

CLUJ POLYNOMIAL IN (4,4), (6,3) AND ((4,8)3) COVERED TORI

In bipartite regular toroidal objects of (4,4), (6,3) and ((4,8)3) tessellation [26,27] (Figure 2) the Cluj and related polynomials (*i.e.*, polynomials counting non-equidistant vertices) and their indices show very simple forms, as given in Table 1. The formulas were obtained by cutting procedures similar to that presented in the introductory section. Note that the studied tori are non-twisted and (with some exceptions) all-even parity of the net parameters [*c*,*n*].

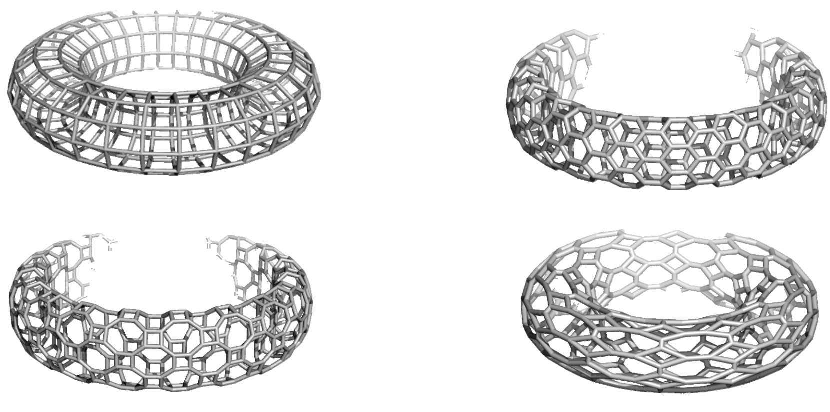


Figure 2. Tori of (4,4); (6,3) (top row) and ((4,8)3)S, ((4,8)3)R (bottom row) covering.

Table 1. Cluj counting polynomials and indices in regular toroidal structures.

$$CJS(x) = e(x^{v/2} + x^{v/2}) \qquad CJP(x) = SZ(x) = e(x^{v/2 \cdot v/2})$$

$$CJS'(1) = e(v/2 + v/2) = e \cdot v = 2(cn)^2 \qquad CJP'(1) = e(v/2 \cdot v/2) = e(v/2)^2$$

$$PI_v(x) = e(x^{v/2+v/2}) = e \cdot x^v \qquad = (1/2)v^3 = (1/2)(cn)^3$$

$$PI_v'(1) = e \cdot v = CJ_eS'(1) \qquad v = cn\,;\; e = (d/2)v$$

[*c*,*n*]	*v*	*e*	***PI**v*(*x*)	***CJS***(***x***)	***CJS'***(1)	***SZ'***(1)
(4,4); d=4						
10,10	100	200	$200x^{100}$	$400x^{50}$	20000	500000
12,14	168	336	$336x^{168}$	$672x^{84}$	56448	2370816
10,20	200	400	$400x^{200}$	$800x^{100}$	80000	4000000
10,50	500	1000	$1000x^{500}$	$2000x^{250}$	500000	62500000
(6,3); d=3						
H 8,8	64	96	$96x^{64}$	$192x^{32}$	6144	98304
H 8,10	80	120	$120x^{80}$	$240x^{40}$	9600	192000
V 8,26	208	312	$312x^{208}$	$624x^{104}$	64896	3374592
V 8,32	256	384	$384x^{256}$	$768x^{128}$	98304	6291456

[*c,n*]	*v*	*e*	$PI_v(x)$	*CJS*(*x*)	*CJS'*(1)	*SZ'*(1)
((4,8)3)S; d=3						
20,20 (*m*=1)	400	600	$600x^{400}$	$1200x^{200}$	240000	24000000
28,42 (*m*=1)	1176	1764	$1764x^{1176}$	$3528x^{588}$	2074464	609892416
5, 10 (*m*=8)[a]	400	600	$600x^{400}$	$1200x^{200}$	240000	24000000
7, 21 (*m*=8)[a]	1176	1764	$1764x^{1176}$	$3528x^{588}$	2074464	609892416
((4,8)3)R; d=3						
10,10 (*m*=4)	400	600	$600x^{400}$	$1200x^{200}$	240000	24000000
10,20 (*m*=4)	800	1200	$1200x^{800}$	$2400x^{400}$	960000	192000000
14,21 (*m*=4)[b]	1176	1764	$294x^{1176} + 1176x^{1162} + 294x^{1148}$	$1764x^{588} + 1764x^{574}$	2049768	595428792

[a] net design by Le_{22tt}; (*m*=8)

[b] net designed by Le; (*m*=4); in case *c,n*=odd, the graph is non-bipartite

CLUJ POLYNOMIAL IN NAPHTHYLENIC TORI

The naphthylenic pattern [28,29] is an analogue of phenylenic (6,4) pattern [30-32] it shows the ring sequence (6,6,4). Naphthylenic structures can be designed either by a cutting procedure (see above) or by using the map operation sequence: *Le*(*Le*(G)), applied on the square tessellation (4,4) embedded in the torus [28,29] We stress that Leapfrog *Le* operation performed on (4,4) results in the ((4,8)3)R tessellation, with the quadrilaterals disposed as rhombs R. A second iteration of *Le* operation will provide the naphthylenic pattern [28] eventually named H/VNPX, with the local signature: (4,6,8): (0,4,0);(1,3,2);(0,8,0), Figure 3, left.

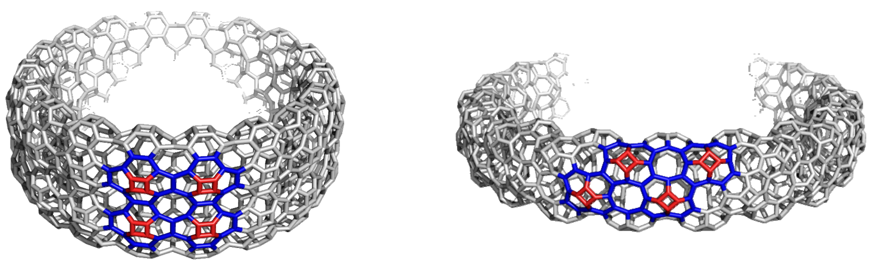


Figure 3. Isomeric *Le*(((4,8)3)R[6,18]) and *Le*(((4,8)3)S[12,36]) objects; *v*=1296; *e*=1944

Formulas to calculate Cluj and related polynomials, and derived indices as well, in toroidal structures designed by *Le*(T((4,8)3)R), are given in Table 2. Examples are given at the bottom of the table.

Table 2. Cluj counting polynomials and indices in *Le*(*Le*(4,4))=*Le*(T((4,8)3)R) toroidal structures; *c*=even; Signature: (4,6,8): (0,4,0);(1,3,2);(0,8,0); *m*=12. (*c*=odd; non-Bipartite)

$$CJS(x) = (v/3)(x^{v/2+[a+18(c-4)/2]} + x^{v/2-[a+18(c-4)/2]}) + (2v/3)(x^{v/2+[13+10(c-4)/2]} + x^{v/2-[13+10(c-4)/2]}) + (v/2)(x^{v/2} + x^{v/2});$$
$$k=1; a=27; \quad k>1; a=31; \quad k=n/c$$
$$CJS'(1) = e \cdot v = (3/2) \cdot v^2 = 216k^2c^4; \quad k=1,2,...$$
$$PI_v(x) = e(x^{v/2+v/2}) = e \cdot x^v$$
$$PI_v'(1) = e \cdot v = CJ_eS'(1)$$
$$CJP(x) = (v/3)(x^{\{v/2+[a+18(c-4)/2]\}\{v/2-[a+18(c-4)/2]\}}) + (2v/3)(x^{\{v/2+[13+10(c-4)/2]\}\{v/2-[13+10(c-4)/2]\}}) + (v/2)(x^{(v/2)^2});$$
$$k=1; a=27; \quad k>1; a=31; \quad k=n/c$$
$$CJP'(1,k>1) = SZ'(1) = 4kc^2(162k^2c^4 - 131c^2 + 230c - 123)$$
$$CJP'(1,k=1) = SZ'(1) = 4c^2(162c^4 - 131c^2 + 302c - 179)$$
$$v = 12kc^2; \quad k = n/c = 1,2,...$$
$$e = (3/2)v$$

(*c*,*n*) *v*; *e*	*CJS*(*x*)	*CJS'*(1)	*SZ'*(1)
(4,8) 384; 576	$128x^{223} + 256x^{205} + 384x^{192} + 256x^{179} + 128x^{161}$	221184	21067392
(6,18) 1296; 1944	$432x^{697} + 864x^{671} + 1296x^{648} + 864x^{625} + 432x^{599}$	2519424	814799088
(8,8) 768; 1152	$256x^{447} + 512x^{417} + 768x^{384} + 512x^{351} + 256x^{321}$	884736	168295680
(10,40) 4800; 7200	$1600x^{2485} + 3200x^{2443} + 4800x^{2400} + 3200x^{2357} + 1600x^{2315}$	34560000	41454523200

When *Le* operation is applied to the ((4,8)3)S tessellation (with the quadrilaterals disposed as squares S) the resulted naphthylenic pattern will show the quadrilaterals disposed as rhombs (Figure 3, right).

As can be seen, the two series show the same tessellation signature (see above) and differ only in the embedding, thus resulting different classes of equivalence and corresponding polynomial terms. The first derivative *CJS*`(1) values are the same in isomeric structures (Tables 2 and 3, the first three rows, next last columns), as a consequence of the bipartity; also it can be considered as a case of (summation operation) degeneracy. In the opposite, the first derivative *SZ*`(1) shows different values (Tables 2 and 3, last columns), the multiplication operation involved being a stronger discriminating operation.

In series *Le*(TH((4,8)3)S), *c*=even, the case *c*=4*m* shows the smallest number of polynomial terms. In series *Le*(TH((4,8)3)R), *c*=even, there is no such a limitation; however, in case *c*=odd of this series, the graphs are non-bipartite and the polynomials show increased number of terms.

Table 3. Cluj counting polynomials and indices in *Le*(TH((4,8)3)S) toroidal structures, *c*=even. Signature: (4,6,8): (0,4,0);(1,3,2);(0,8,0); *m*=3; (*c*=odd; Bipartite)

$$\begin{aligned}
CJS(x) = {} & (v/6)(x^{v/2+[24+15(m-1)+12(k-1)(m+1)]} + x^{v/2-[24+15(m-1)+12(k-1)(m+1)]}) + \\
& (v/3)(x^{v/2+[16+11(m-1)+12(k-1)(m+1)]} + x^{v/2-[16+11(m-1)+12(k-1)(m+1)]}) + \\
& (v/6)(x^{v/2+[12+9(m-1)]} + x^{v/2-[12+9(m-1)]}) + \\
& (v/3)(x^{v/2+[4+5(m-1)]} + x^{v/2-[4+5(m-1)]}) \\
& (v/2)(x^{v/2} + x^{v/2}); \\
& \quad k = n/c; \quad m = (c-4)/4
\end{aligned}$$

$$CJS'(1) = e \cdot v = (3/2) \cdot v^2 = (27/2)k^2c^4; \quad k = 1,2,...$$

$$PI_v(x) = e(x^{v/2+v/2}) = e \cdot x^v$$

$$PI_v'(1) = e \cdot v = CJ_eS'(1)$$

$$\begin{aligned}
CJP(x) = {} & (v/6)(x^{\{v/2+[24+15(m-1)+12(k-1)(m+1)]\} \cdot \{v/2-[24+15(m-1)+12(k-1)(m+1)]\}}) + \\
& (v/3)(x^{\{v/2+[16+11(m-1)+12(k-1)(m+1)]\} \cdot \{v/2-[16+11(m-1)+12(k-1)(m+1)]\}}) + \\
& (v/6)(x^{\{v/2+[12+9(m-1)]\} \cdot \{v/2-[12+9(m-1)]\}}) + \\
& (v/3)(x^{\{v/2+[4+5(m-1)]\} \cdot \{v/2-[4+5(m-1)]\}}) \\
& (v/2)(x^{(v/2) \cdot (v/2)}); \\
& \quad k = n/c; \quad m = (c-4)/4
\end{aligned}$$

$$\begin{aligned}
CJP'(1) = SZ'(1) = {} & (kc^2/16)(162k^2c^4 - 216k^2c^2 - 12kc^2 - 71c^2 + \\
& 864kc + 480c - 1728)
\end{aligned}$$

$$v = 3kc^2; \quad k = n/c = 1,2,...$$

$$e = (3/2)v$$

(*c*,*n*) *v; e*	*CJS*(*x*)	*CJS'*(1)	*SZ'*(1)
(8,16) 384; 576	$64x^{240} + 128x^{232} + 64x^{204} + 128x^{196} + 384x^{192} + 128x^{188} + 64x^{180} + 128x^{152} + 64x^{144}$	221184	20870144
(12,36) 1296; 1944	$216x^{759} + 432x^{747} + 216x^{669} + 432x^{657} + 1296x^{648} + 432x^{639} + 216x^{627} + 432x^{549} + 216x^{537}$	2519424	809267760
(16,16) 768; 1152	$128x^{438} + 256x^{422} + 128x^{414} + 256x^{398} + 768x^{384} + 256x^{370} + 128x^{354} + 256x^{346} + 128x^{330}$	884736	168961024

CLUJ POLYNOMIAL IN TiO_2 TORI

After the discovery of carbon nanotubes many researchers addressed the question about the possible existence of nano-tubular forms of other elements and they tried to obtain inorganic nanostructures [33-35]. Among numerous oxide nanostructures, the titanium nanotubular materials are of high interest due to their chemical inertness, endurance, strong oxidizing power, large surface area, high photocatalytic activity, non-toxicity and low production cost. The application of TiO_2 nanotubes to photocatalysis, in solar cells, as nanoscale materials for lithium-ion batteries and as gas-sensing material was discussed in the literature [36-42]. The nanotubes were synthesized using various precursors [41-47], carbon nanotubes, porous alumina or polymer membranes as templates [40-56] fabrication by anodic oxidation of Ti [57-59], sol–gel technique [60-64] and sono-chemical synthesis [65]. Models of possible growth mechanisms of titanium nanotubes are discussed [48,49,64] but the details of the atomic structure of the nanotube walls and their stacking mode are unknown. TiO_2 nanotubes are semiconductors with a wide band gap and their stability increases with increasing of their diameters. The numerous studies for the use of nanotubular titania in technological applications require a lot of theoretical studies of stability and other properties of such structures. Theoretical studies on the stability and electronic characteristics of TiO_2 nanostructures were presented in ref. [66-68].

The titanium nanostructures on study below can be achieved by map operations: the sequence consists of *Du*[*Med*(*G*)], applied on polyhex tori or tubes (Figure 4).

Formulas for calculating Cluj and related polynomials, in toroidal TiO_2 structures, are given in Table 4.

Figure 4. TiO_2 covering embedded in the torus, designed by *Du*(*Med*(H(6,3)[*c*,*n*]))

Table 4. Cluj and Related Polynomials in TiO_2 Tori

$CJS(x) = e(x^{e_{ka}} + x^{e_{kb}})$	$v = (3/2)cn$
$CJS'(1) = e(e_{ka} + e_{kb}) = e \cdot v = (1/2)e^2$	$e = 3cn$
$PI_v(x) = e(x^{e_{ka}+e_{kb}}) = e \cdot x^v$	$e_{ka} = e_1 k + (k-1)(c/2)$
$PI_v'(1) = e(e_{ka} + e_{kb}) = e \cdot v = CJ_eS'(1)$	$e_{kb} = e_{ka} + c$
$CJP(x) = SZ(x) = e(x^{e_{ka} \cdot e_{kb}})$	$e_1 = c^2 - (c/2) \cdot (c/2+1)$
$CJP'(1) = e(e_{ka} \cdot e_{kb}) = e(c/4)^2(3n-2)(3n+2)$	$k = n/c$

Tori	***CJS***(*x*)	***CJS`***(1)	***CJP***(*x*)	***CJP`***(1)
H[10,10]	$300x^{70}+300x^{80}$	45000	$300x^{5600}$	1680000
H[10,20]	$600x^{145}+600x^{155}$	180000	$600x^{22475}$	13485000
H[10,30]	$900x^{220} + 900x^{230}$	405000	$900x^{50600}$	45540000
H[12,14]	$504x^{120} + 504x^{132}$	127008	$504x^{15840}$	7983360
V[8,10]	$240x^{56} + 240x^{64}$	28800	$240x^{3584}$	860160
V[10,20]	$600x^{145}+600x^{155}$	180000	$600x^{22475}$	13485000
V[10,30]	$900x^{220}+900x^{230}$	405000	$900x^{50600}$	45540000
V[10,50]	$1500x^{370}+1500x^{380}$	1125000	$1500x^{140600}$	210900000

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