Generation of Structures in Chemistry and Mathematics

Public Defense

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Combinatorial Algorithms and Algorithmic Graph Theory
Department of Applied Mathematics and Computer Science
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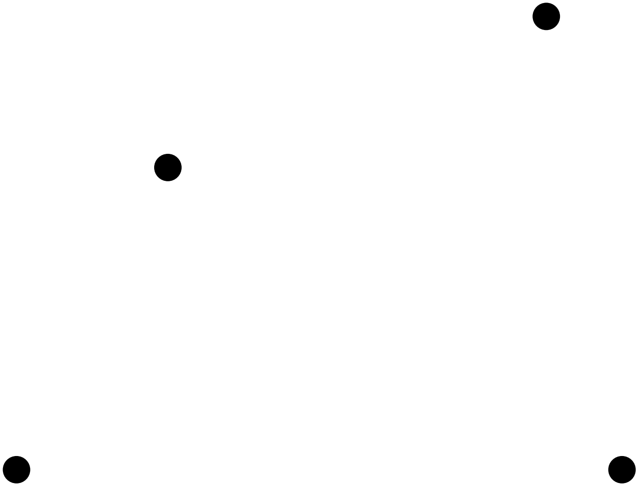
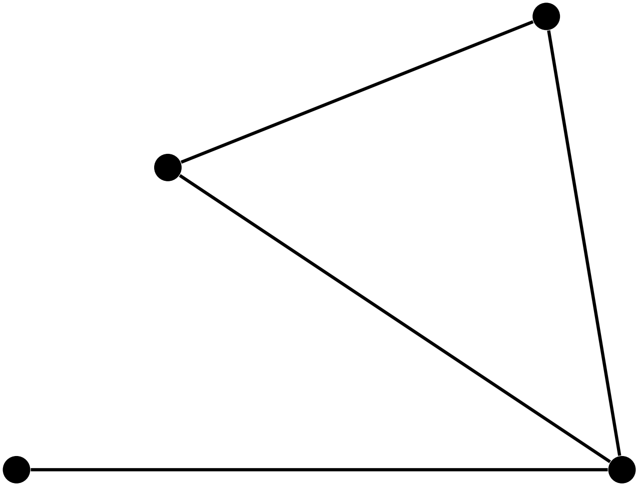
Overview

1. Concepts
   1. Graphs / Chemical graphs
   2. Tilings
   3. Generation algorithms
2. Short
   1. Generalized cubic graphs
   2. Delaney-Dress symbols
   3. Azulenoids
3. Detailed
   1. Nanocones

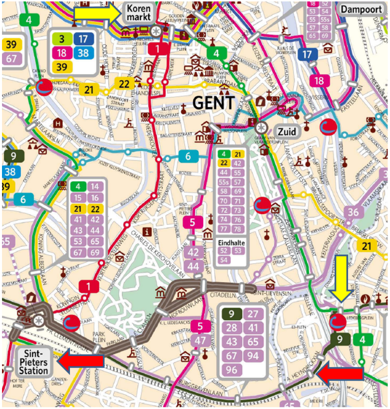
Graph

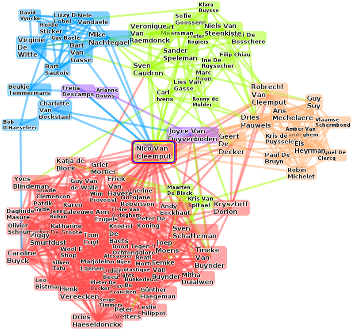


Graph

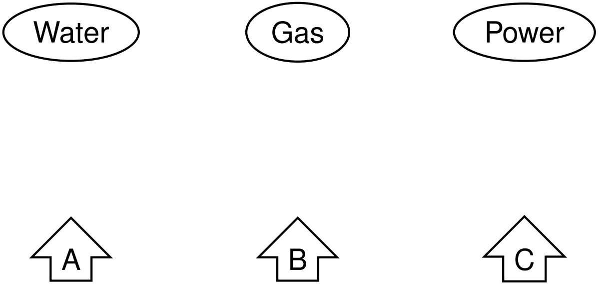


Graphs are everywhere

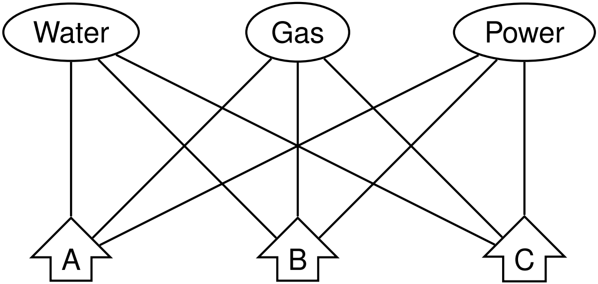




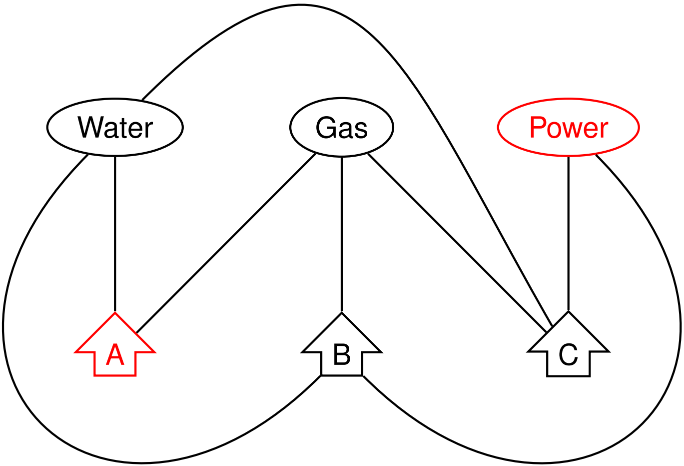
Three utilities



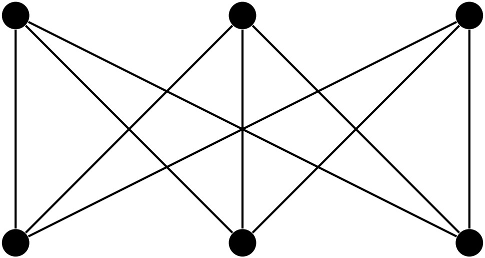
Three utilities



Three utilities

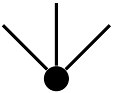


Three utilities

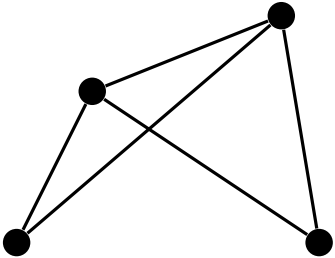


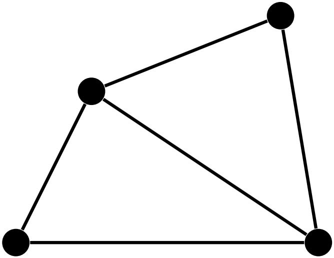
$K_{3,3}$ is not planar

3

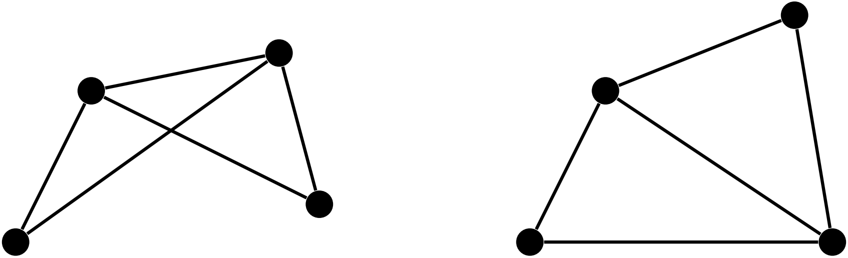


Isomorphism





Isomorphism



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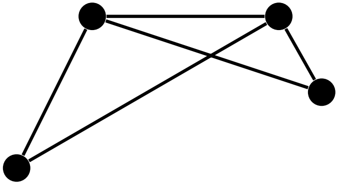

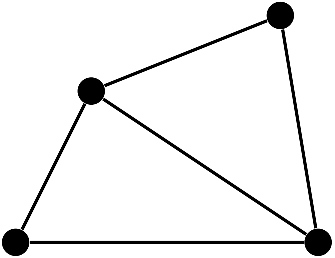

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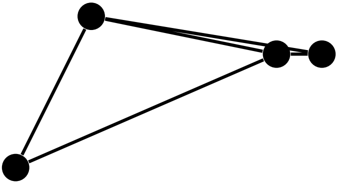

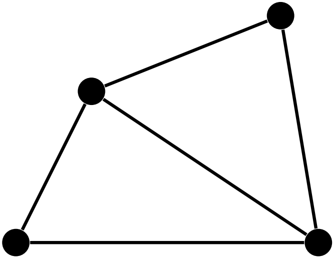

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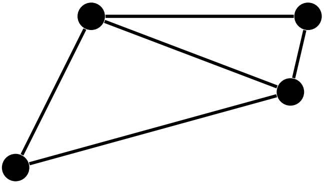

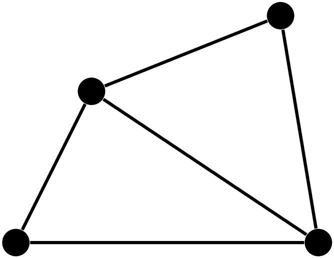

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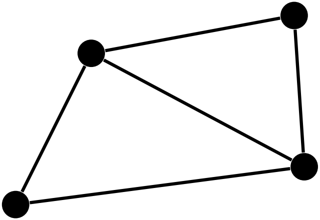

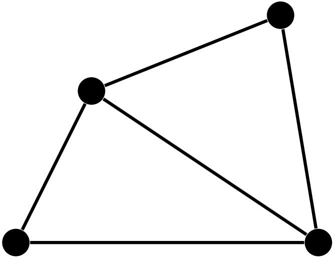

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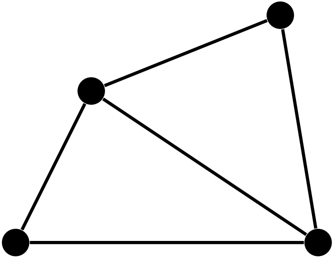

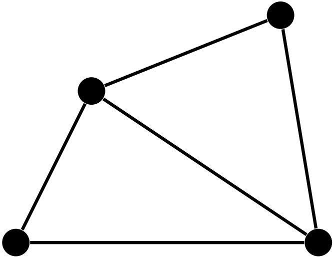

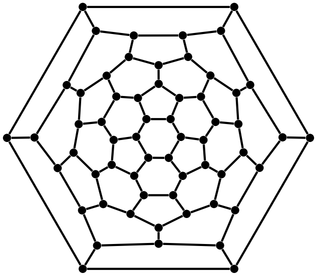

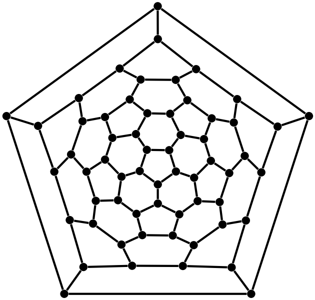

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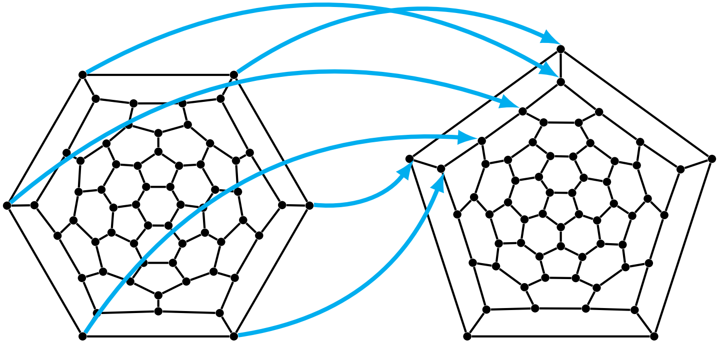
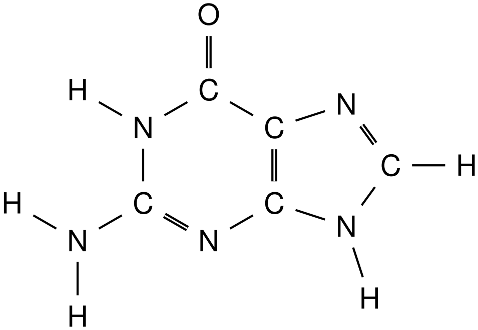
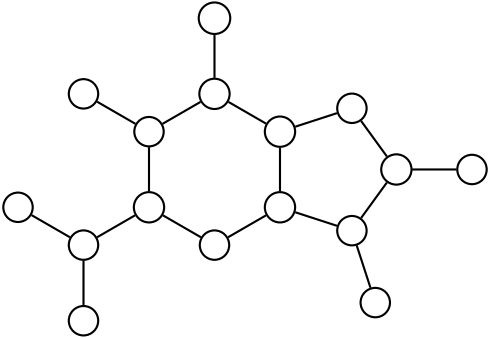


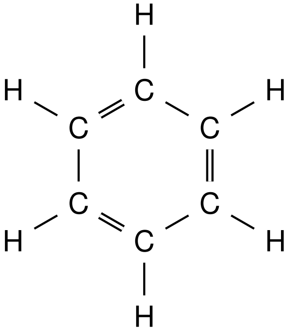
Chemical graph theory



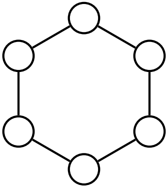
Chemical graph theory

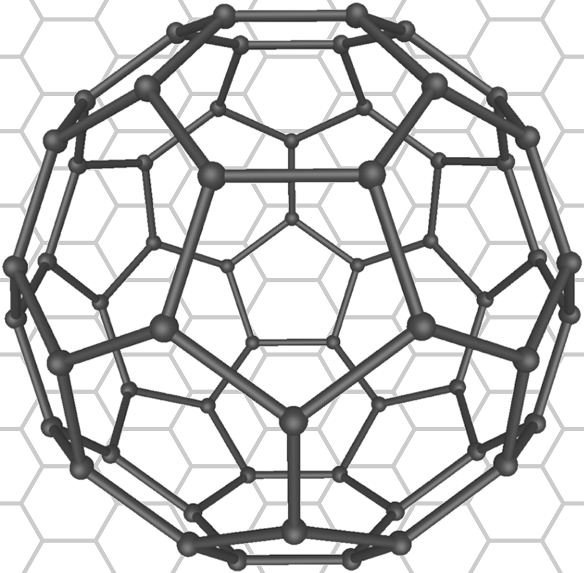


Chemical graph theory



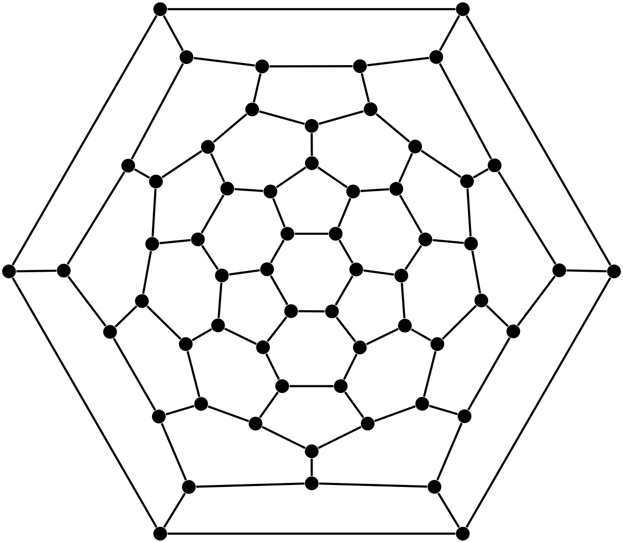
Chemical graph theory





Buckminsterfullerene

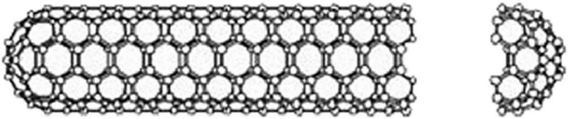
Kroto, Curl and Smalley (1985/Nobel Prize 1996)
truncated icosahedron
12 pentagons and 20 hexagons
planar

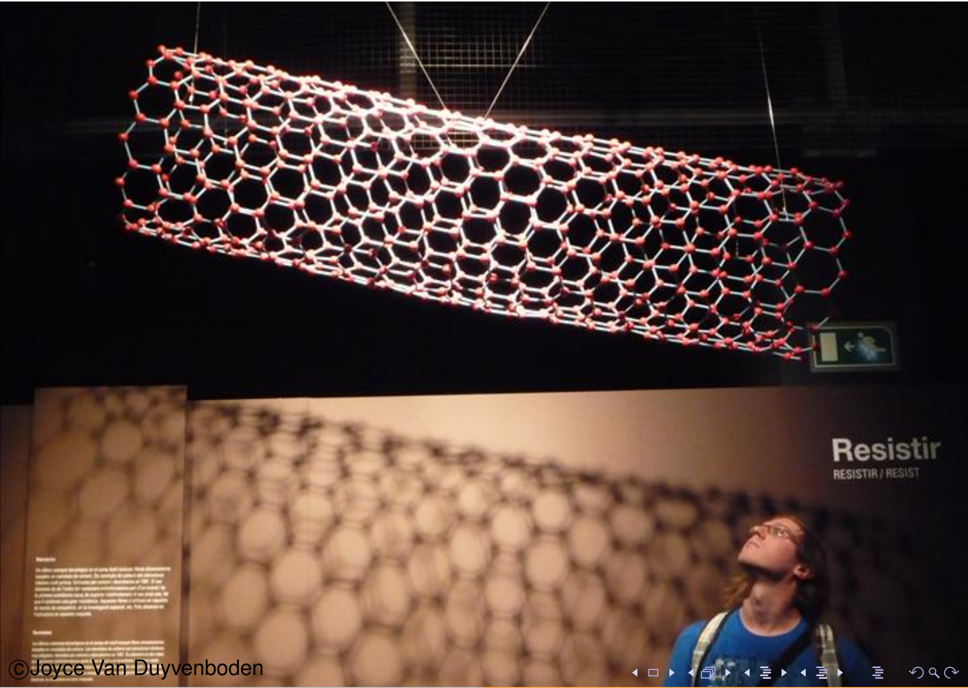


Fullerenes

carbon molecules
12 pentagons
3-regular
planar

Nanotubes





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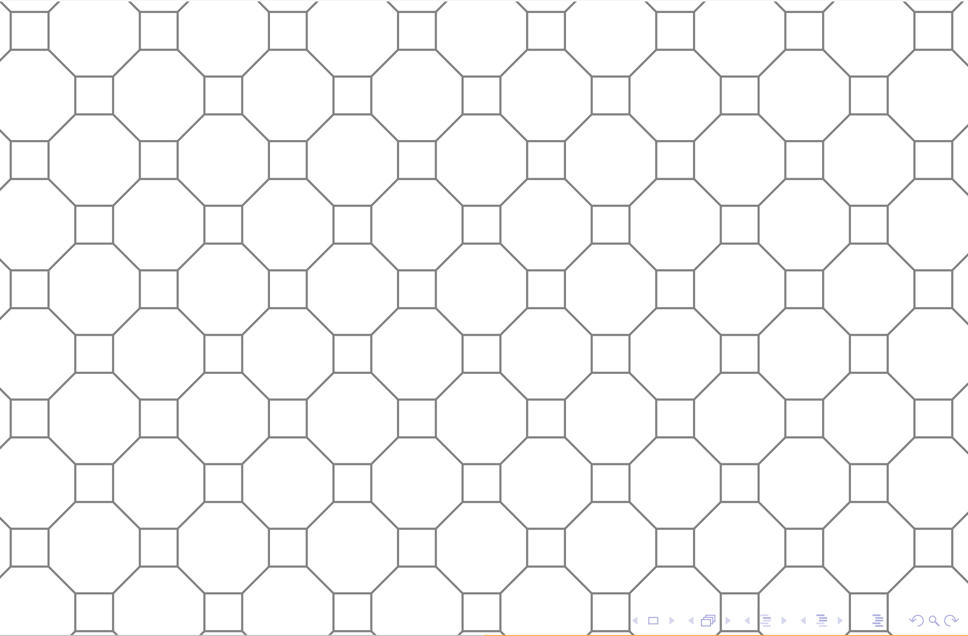
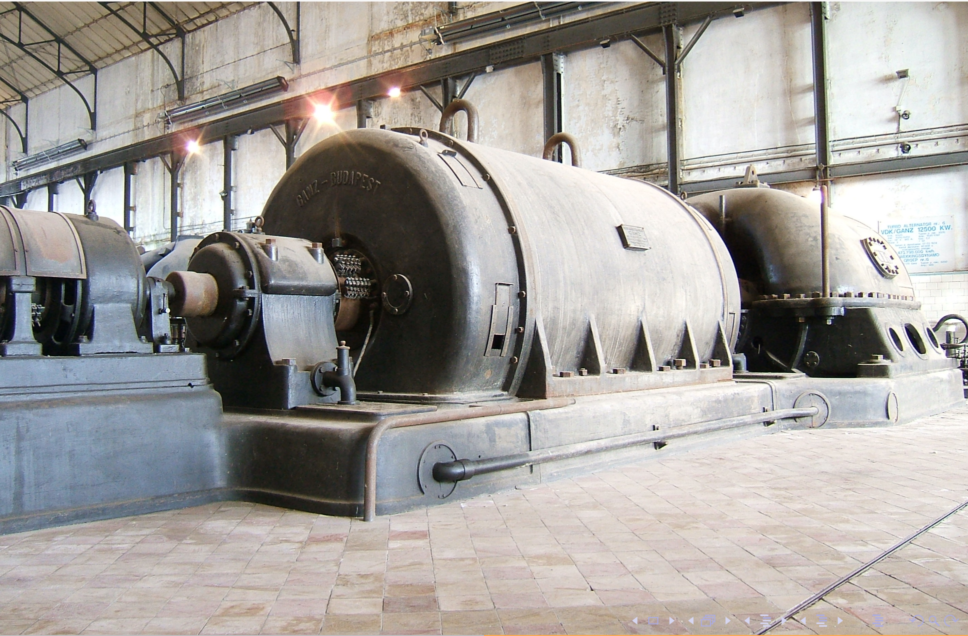
Tilings



Generator



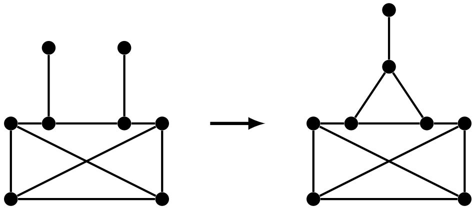
Generator

Even numbers from 1 to 10

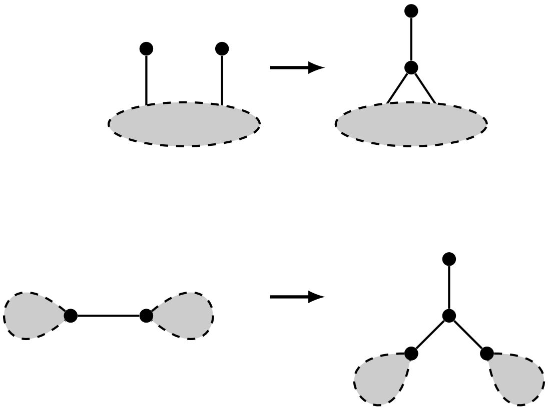
Random generation algorithm:
2, 6, 6, 8, 2

Exhaustive, isomorphism-free generation algorithm :
6, 8, 4, 2, 10

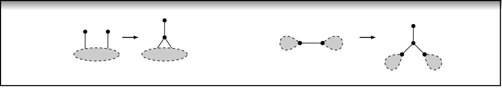
Construction operations

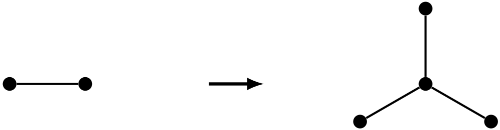


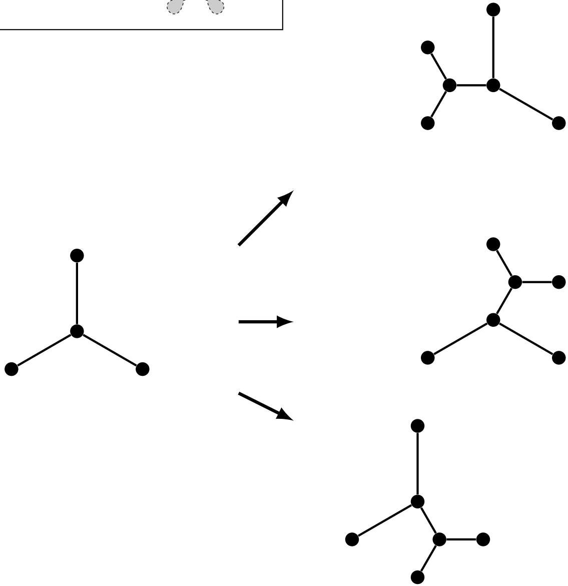
Construction operations

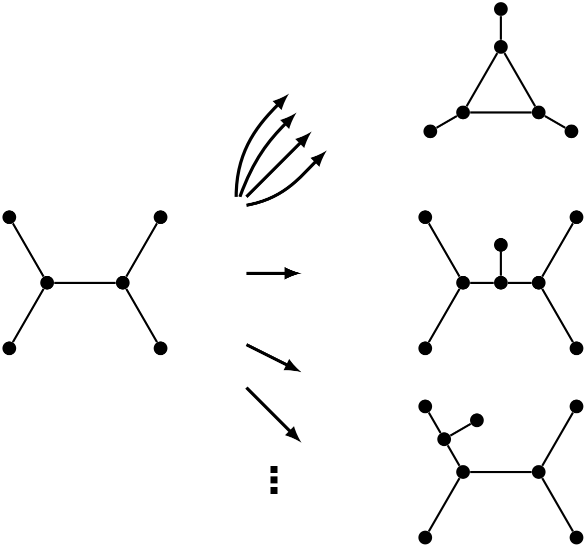


Generate all simple graphs with degrees 1 and 3









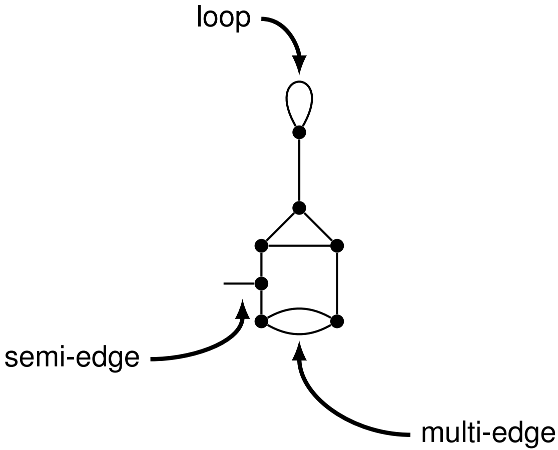
Avoiding isomorphic copies

- isomorphism rejection by list
- canonical representatives and
  Read/Faradžev-type orderly algorithms
- McKay's canonical construction path method
- homomorphism principle
- double coset method
- ...

Overview

- Generalized cubic graphs
- Delaney-Dress symbols
- Azulenoids
- Nanocones

Generalized cubic graphs



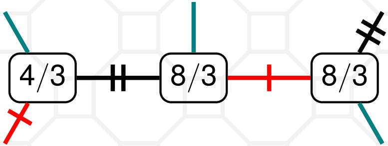
n	$\mathcal{C}$	$\mathcal{L}$	$\mathcal{S}$	$\mathcal{M}$	$\mathcal{LS}$	$\mathcal{LM}$	$\mathcal{SM}$	$\mathcal{P}$
1	**0**	**0**	**1**	**0**	**2**	**0**	**1**	**2**
2	**0**	**1**	**1**	**1**	**3**	**2**	**3**	**5**
3	**0**	**0**	**2**	**0**	**4**	**0**	**4**	**7**
4	**1**	**2**	**6**	**2**	**12**	**5**	**12**	**22**
5	**0**	**0**	**10**	**0**	**22**	**0**	**22**	**43**
6	**2**	**6**	**29**	**6**	**68**	**17**	**68**	**141**
7	**0**	**0**	**64**	**0**	**166**	**0**	**166**	**373**
8	**5**	**20**	**194**	**20**	**534**	**71**	**534**	**1 270**
9	**0**	**0**	**531**	**0**	**1 589**	**0**	**1 589**	**4 053**
10	**19**	**91**	**1 733**	**91**	**5 464**	**388**	**5 464**	**14 671**
11	**0**	**0**	**5 524**	**0**	**18 579**	**0**	**18 579**	**52 826**
12	**85**	**509**	**19 430**	**509**	**68 320**	**2 592**	**68 320**	**203 289**
13	**0**	**0**	**69 322**	**0**	**255 424**	**0**	**255 424**	**795 581**
14	**509**	**3 608**	**262 044**	**3 608**	**1 000 852**	**21 096**	**1 000 852**	**3 241 367**
15	**0**	**0**	**1 016 740**	**0**	**4 018 156**	**0**	**4 018 156**	**13 504 130**
16	**4 060**	**31 856**	**4 101 318**	**31 856**	**16 671 976**	**204 638**	**16 671 976**	**57 904 671**
17	**0**	**0**	**16 996 157**	**0**	**70 890 940**	**0**	**70 890 940**	**253 856 990**
18	**41 301**	**340 416**	**72 556 640**	**340 416**	**309 439 942**	**2 317 172**	**309 439 942**	**1 139 231 977**
19	**0**	0	317 558 689	0	1 381 815 168	0	1 381 815 168	5 219 113 084
20	**510 489**	4 269 971	1 424 644 848	4 269 971	6 310 880 471	30 024 276	6 310 880 471	24 401 837 085
21	**0**	0	6 536 588 420	0	29 428 287 639	0	29 428 287 639	116 278 408 069
22	**7 319 447**	61 133 757	30 647 561 117	61 133 757	140 012 980 007	437 469 859	140 012 980 007	564 380 686 932
23	**0**	0	146 647 344 812	0		0		
24	**117 940 535**	978 098 997		978 098 997		7 067 109 598		

n	$\mathcal{C}$	$\mathcal{L}$	$\mathcal{S}$	$\mathcal{M}$	$\mathcal{LS}$	$\mathcal{LM}$	$\mathcal{SM}$	$\mathcal{P}$
10	0.0s	0.0s	0.0s	0.0s	0.1s	0.0s	0.1s	0.1s
11	0.0s	0.0s	0.1s	0.0s	0.2s	0.0s	0.3s	0.4s
12	0.0s	0.0s	0.6s	0.0s	0.8s	0.0s	1.3s	1.8s
13	0.0s	0.0s	2.2s	0.0s	3.5s	0.0s	5.4s	7.4s
14	0.0s	0.0s	9.1s	0.1s	14.9s	0.2s	22.6s	32.2s
15	0.0s	0.0s	37.3s	0.0s	64.1s	0.0s	97.2s	$\approx$ 2m
16	0.0s	0.3s	$\approx$ 2m	0.5s	$\approx$ 4m	2.5s	$\approx$ 7m	$\approx$ 11m
17	0.0s	0.0s	$\approx$ 11m	0.0s	$\approx$ 22m	0.0s	$\approx$ 32m	$\approx$ 53m
18	0.1s	3.0s	$\approx$ 53m	5.1s	$\approx$ 1h	31.0s	$\approx$ 2h	$\approx$ 4h
19	0.0s	0.0s	$\approx$ 3h	0.0s	$\approx$ 9h	0.0s	$\approx$ 11h	$\approx$ 21h
20	1.4s	39.0s	$\approx$ 18h	67.9s	$\approx$ 45h	$\approx$ 7m	$\approx$ 56h	$\approx$ 4 days
21	0.0s	0.0s	$\approx$ 3 days	0.0s	$\approx$ 9 days	0.0s	$\approx$ 11 days	$\approx$ 24 days
22	18.6s	$\approx$ 9m	$\approx$ 18 days	$\approx$ 17m	$\approx$ 52 days	$\approx$ 1h	$\approx$ 57 days	$\approx$ 132 days
23	0.0s	0.0s	$\approx$ 93 days	0.0s		0.0s		
24	$\approx$ 4m	$\approx$ 2h		$\approx$ 5h		$\approx$ 34h		

n	$\mathcal{L}$	$\mathcal{S}$	$\mathcal{M}$	$\mathcal{LS}$	$\mathcal{LM}$	$\mathcal{SM}$	$\mathcal{P}$
20	109 486.4/s	21 018.1/s	62 886.2/s	38 402.7/s	67 943.6/s	31 064.8/s	60 348.0/s
21		19 815.3/s		34 481.1/s		29 498.9/s	54 640.6/s
22	105 914.3/s	18 828.6/s	58 551.6/s	30 776.7/s	61 977.7/s	28 084.3/s	49 331.1/s
23		181 31.0/s					
24	101 667.2/s		54 271.3/s		56 704.4/s		

Delaney-Dress symbols

Finite, discrete encoding of a periodic tiling

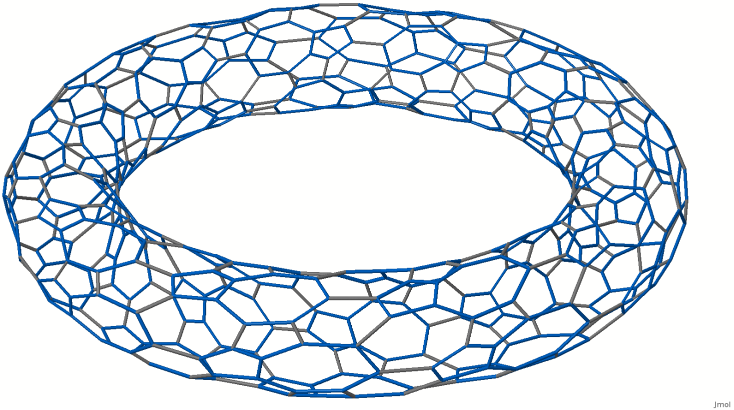


n	C_4^q-markable	ddgraphs	pregraphs
1	1	0.0s	0.0s
2	3	0.0s	0.0s
3	2	0.0s	0.0s
4	9	0.0s	0.0s
5	7	0.0s	0.0s
6	29	0.0s	0.0s
7	27	0.0s	0.0s
8	105	0.0s	0.0s
9	118	0.0s	0.0s
10	392	0.0s	0.1s
11	546	0.0s	0.3s
12	1 722	0.1s	1.3s
13	2 701	0.1s	5.2s
14	7 953	0.3s	22.0s
15	13 966	0.4s	94.8s
16	40 035	1.5s	$\approx$ 7m
17	75 341	2.2s	$\approx$ 31m
18	210 763	8.0s	$\approx$ 2h
19	420 422	14.0s	$\approx$ 11h
20	1 162 192	46.6s	$\approx$ 56h
21	2 419 060	86.7s	
22	6 626 608	$\approx$ 4m	
23	14 292 180	$\approx$ 9m	
24	38 958 567	$\approx$ 28m	
25	86 488 183	$\approx$ 59m	
26	235 004 258	$\approx$ 2h	
27	534 796 010	$\approx$ 6h	
28	1 450 990 711	$\approx$ 19h	
29	3 373 088 492	$\approx$ 43h	
30	9 147 869 418	$\approx$ 5 days	

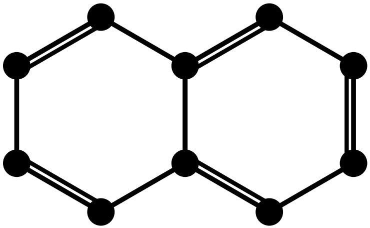
n	Delaney-Dress graphs	time	rate
1	1	0.0s	
2	7	0.0s	
3	3	0.0s	
4	22	0.0s	
5	13	0.0s	
6	70	0.0s	
7	67	0.0s	
8	315	0.0s	
9	393	0.0s	
10	1 577	0.0s	
11	2 515	0.0s	
12	9 480	0.1s	94 800.00/s
13	17 205	0.1s	172 050.00/s
14	61 594	0.3s	205 313.33/s
15	123 953	0.4s	309 882.50/s
16	433 030	1.6s	270 643.75/s
17	931 729	2.5s	372 691.60/s
18	3 196 841	9.1s	351 301.21/s
19	7 258 011	16.3s	445 276.75/s
20	24 630 262	55.0s	447 822.95/s
21	58 309 071	105.9s	550 605.01/s
22	196 266 434	$\approx$ 5m	568 064.93/s
23	481 330 615	$\approx$ 12m	666 478.28/s
24	1 610 942 856	$\approx$ 38m	691 629.25/s
25	4 071 117 829	$\approx$ 1h	785 187.34/s
26	13 569 014 653	$\approx$ 4h	826 265.50/s
27	35 202 390 477	$\approx$ 10h	919 758.85/s
28	116 994 675 348	$\approx$ 33h	960 576.60/s
29	310 624 700 725	$\approx$ 3 days	1 049 801.45/s
30	1 030 455 432 427	$\approx$ 11 days	1 084 892.06/s

n	Delaney-Dress symbols	time
1	3	0.0s
2	15	0.0s
3	8	0.0s
4	37	0.0s
5	15	0.0s
6	86	0.0s
7	64	0.0s
8	217	0.2s
9	185	0.5s
10	527	3.8s
11	506	13.0s
12	1 597	95.1s
13	1 575	$\approx$ 6m
14	4 227	$\approx$ 42m
15	4 532	$\approx$ 2h
16	12 078	$\approx$ 19h
17	13 105	$\approx$ 3 days
18	34 250	$\approx$ 23 days

Azulenoids

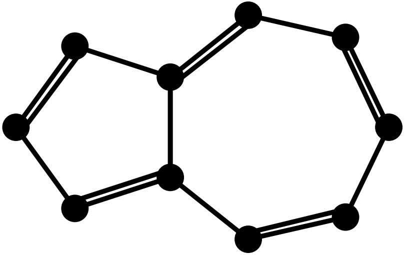


naphtalene



$C_{10}H_8$

azulene



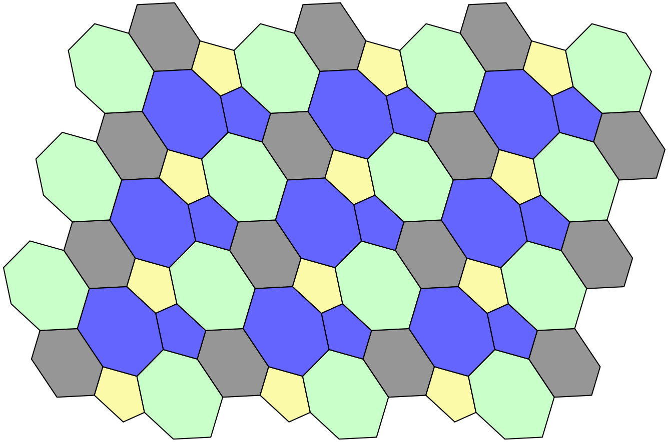
$C_{10}H_8$

Question

We don’t yet know whether and how the electron mobility might manifest itself among azulenes embedded within a toroidal fullerene-style network.

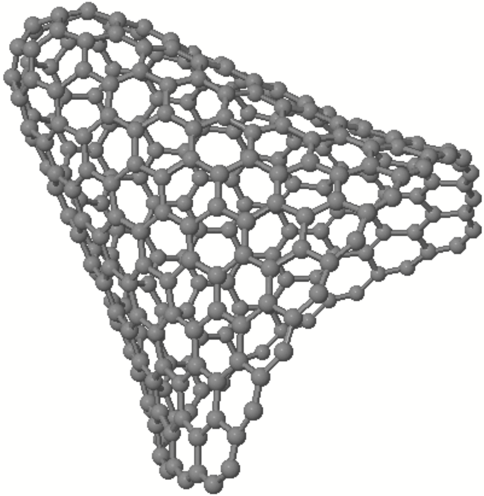
How many variations of such networks are theoretically possible?

Edward Kirby

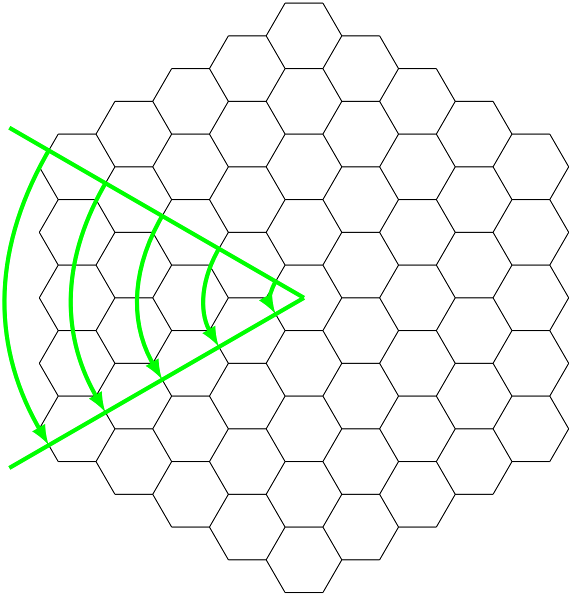


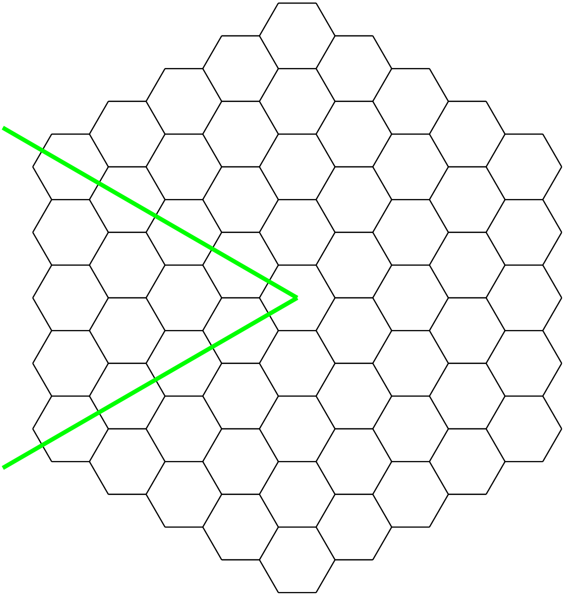
DEMO

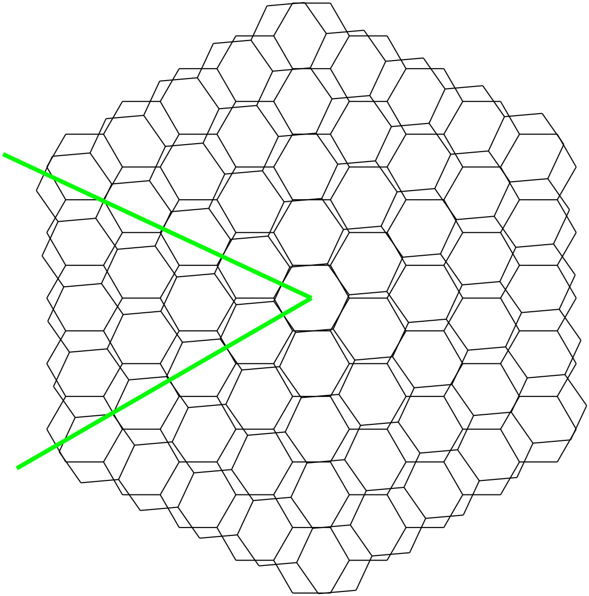
Nanocones

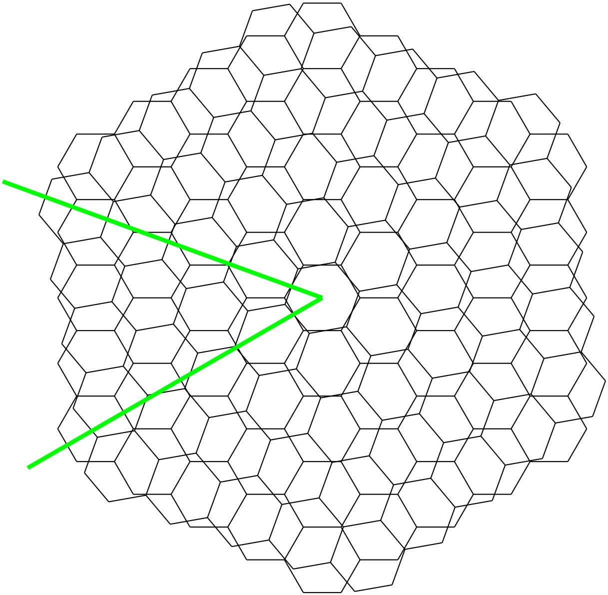


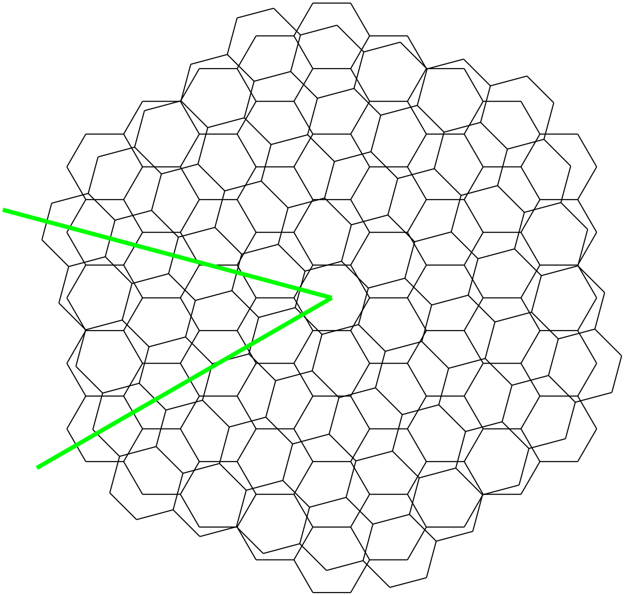
Nón lá

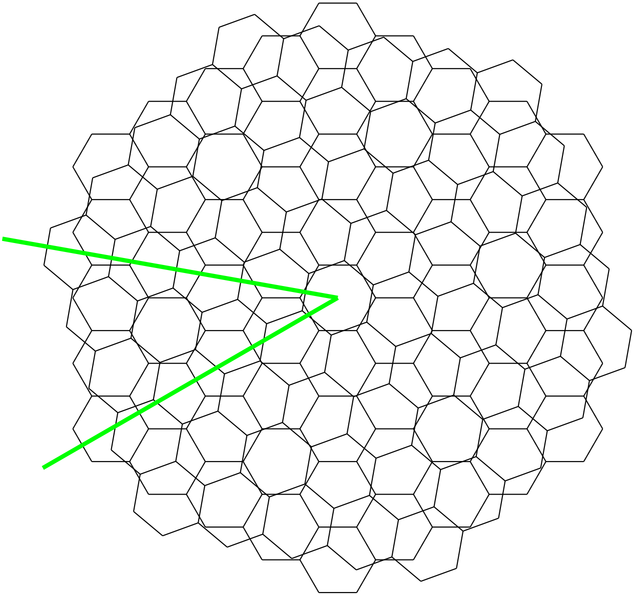


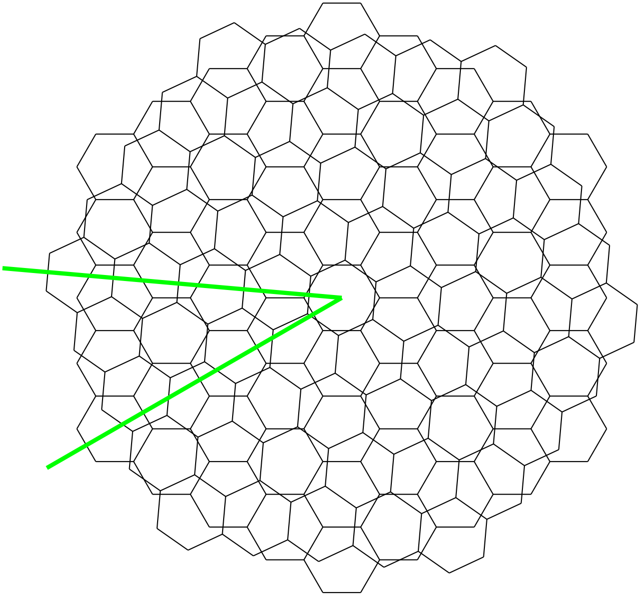


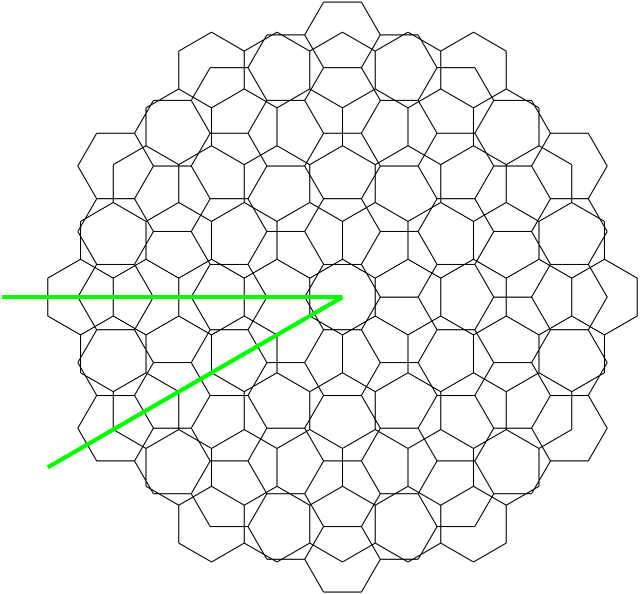


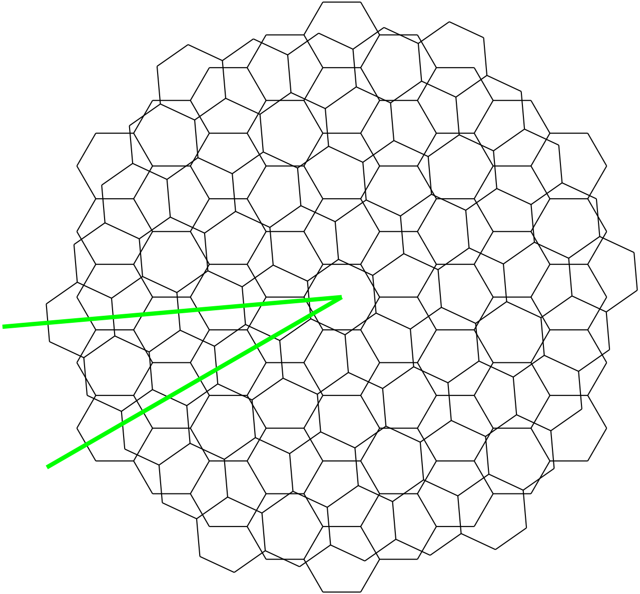


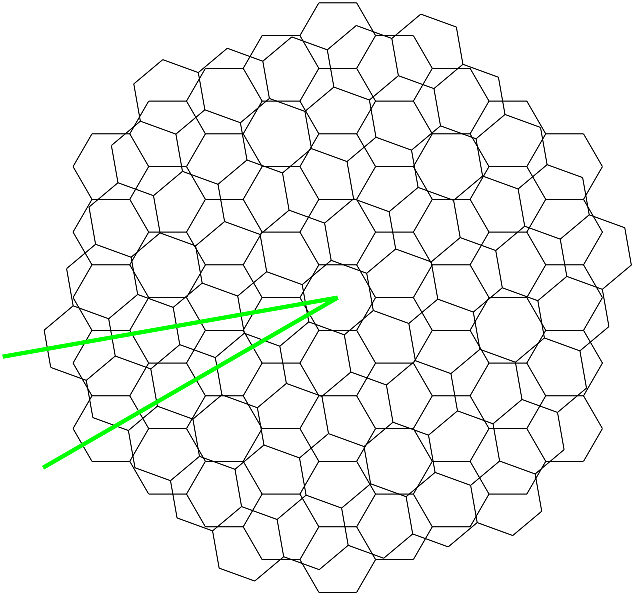


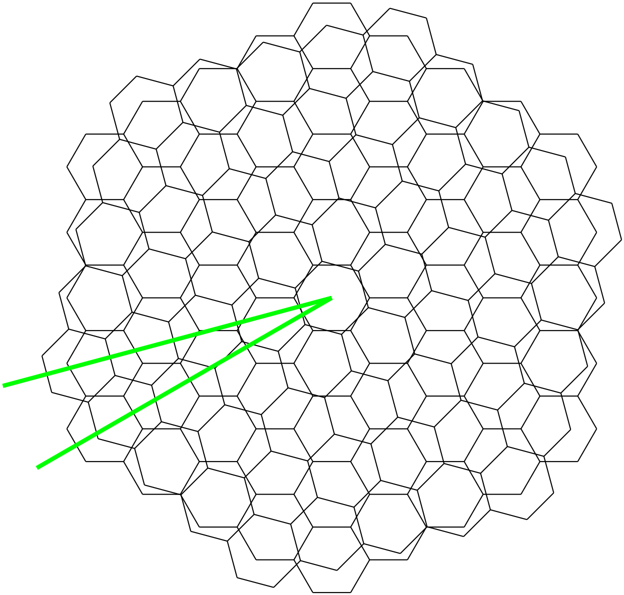


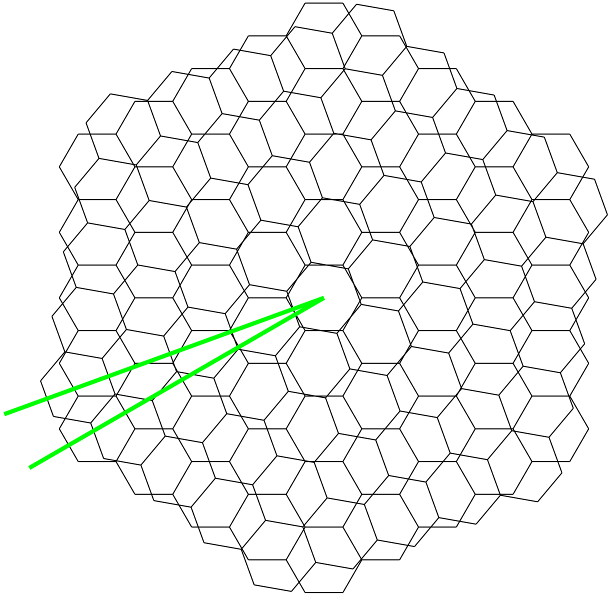


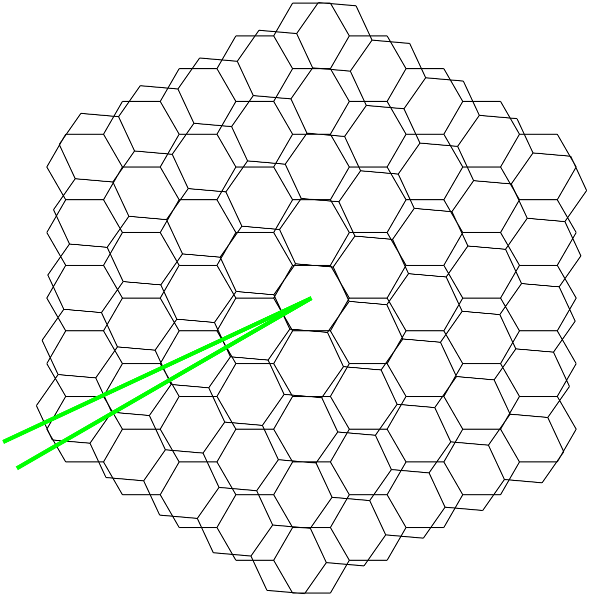


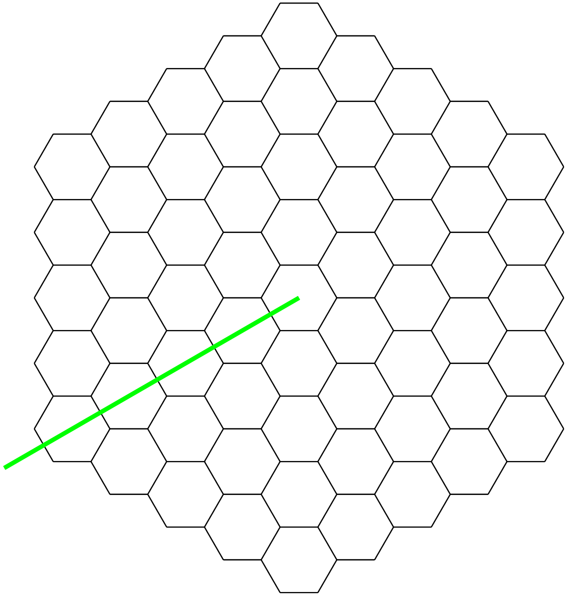


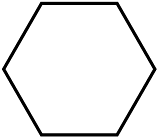


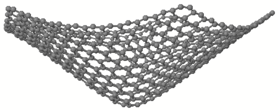


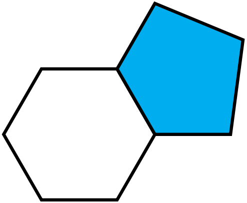


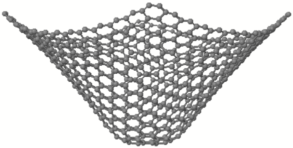


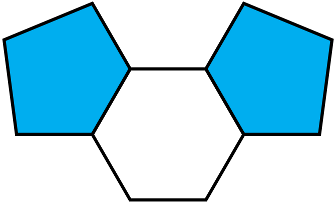


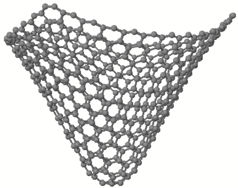


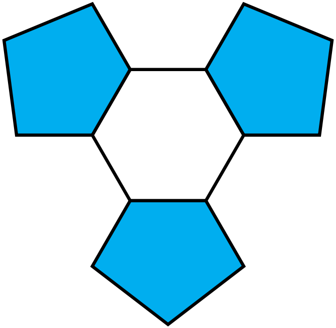


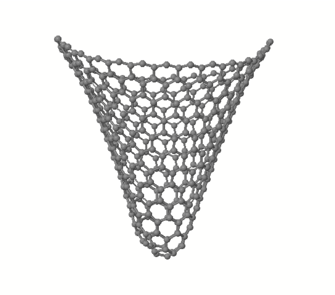


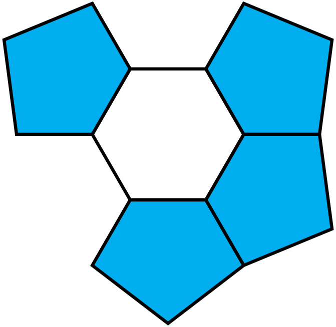


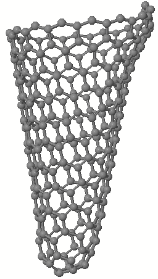


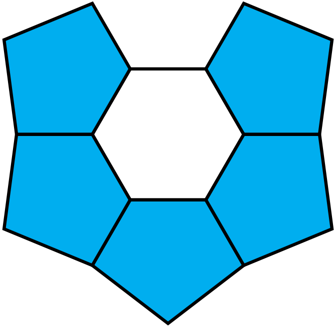


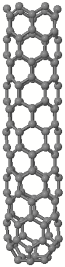


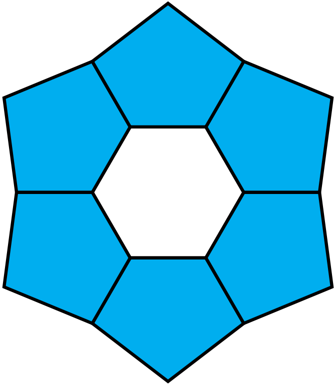




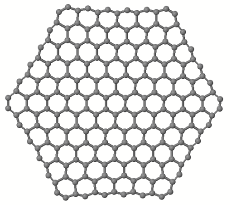




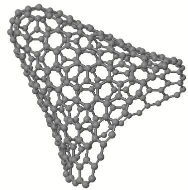




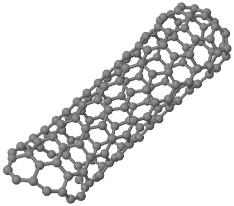
graphene



nanocone

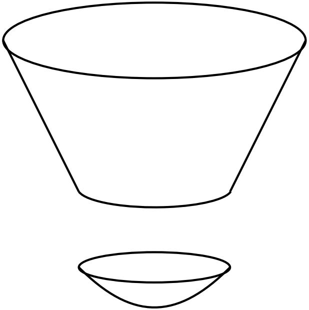


nanotube

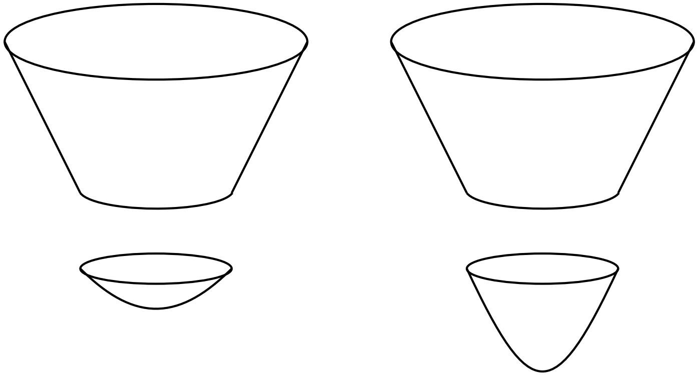


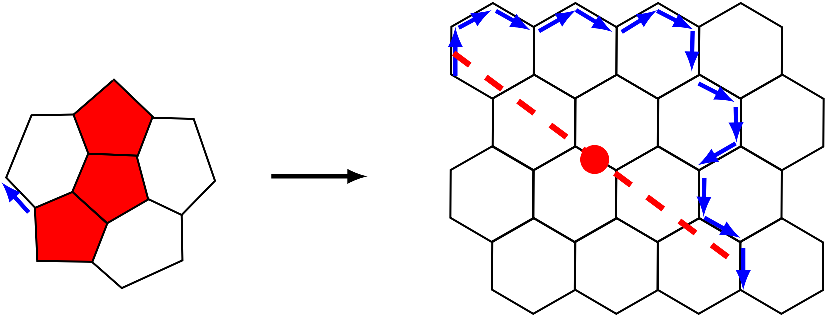
all structures infinite

Coarse classification first done by Balaban and Klein



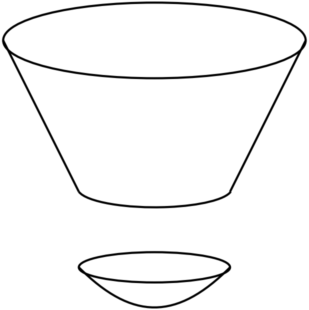
isomorphic $\Rightarrow$ equivalent





rrlrlrrlrrlrl

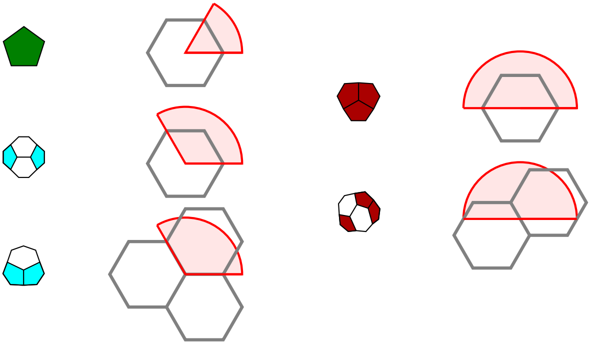
Two nanocones are equivalent if and only if they correspond to the same conjugacy class of rotations.



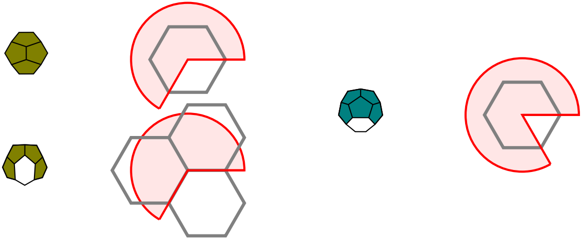
8 possible types

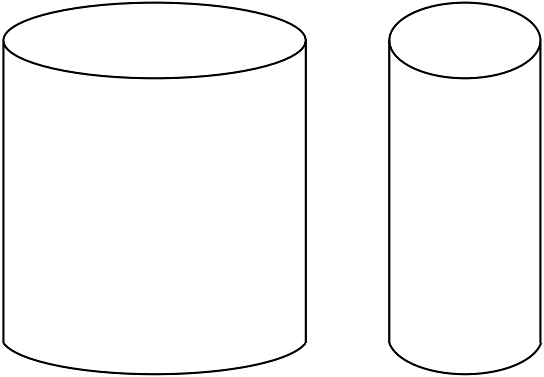
per size finite number of possibilities

Existence of the 8 types

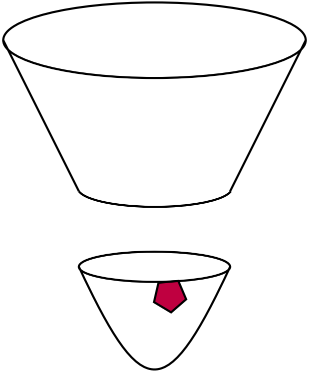


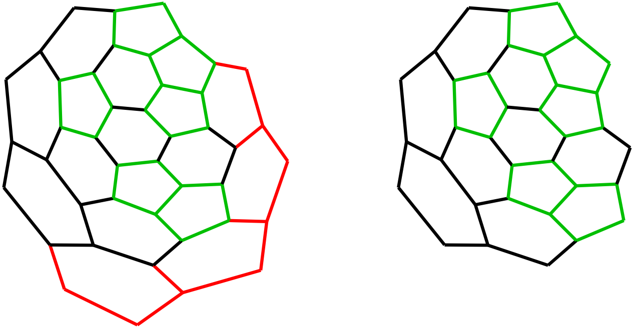
Existence of the 8 types



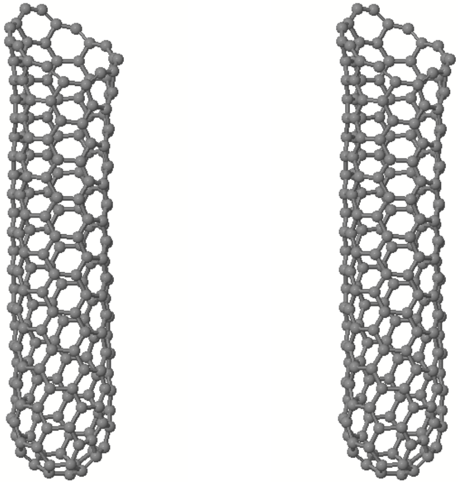


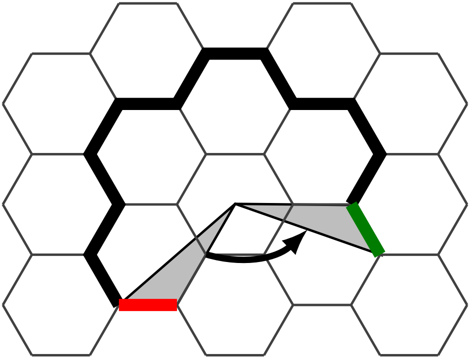
In nanotubes there is an infinite number of these equivalence classes.



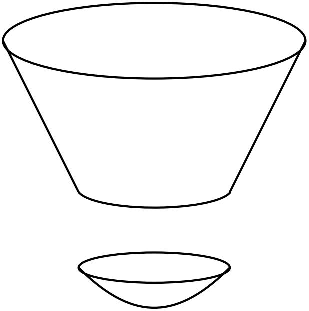


$$rlrlrlrlrlrllrlrlrlr = (rl)^5(lr)^4$$





$$(2n_0+n_1-n_2-2n_3-n_4+n_5)\mathbf{e}_1+(n_0+2n_1+n_2-n_3-2n_4-n_5+1)\mathbf{e}_2$$
$$=$$
$$(m_0+2m_1+m_2-m_3-2m_4-m_5)\mathbf{e}_1+(-m_0+m_1+2m_2+ m_3-m_4-2m_5+1)\mathbf{e}_2$$



Specify type

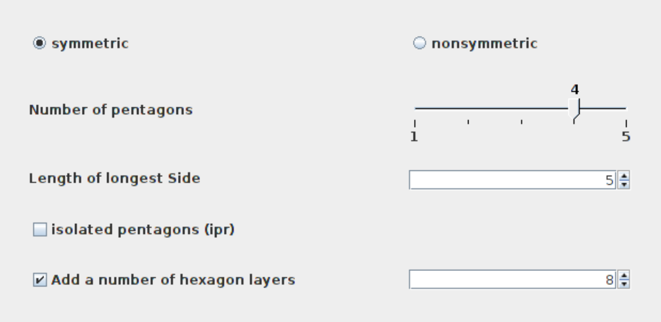
Specify ‘size’

	2 s	2 n	3 s	3 n	4 s	4 n	5
5	3	6	18	63	37	89	1
10	6	11	124	413	975	2 272	212
15	8	16	387	1 288	7 040	16 032	3 941
20	11	21	915	2 960	29 342	65 056	31 025
25	13	26	1 757	5 646	88 918	194 044	150 732
30	16	31	3 039	9 640	220 741	475 422	547 166
35	18	36	4 793	15 138	476 101	1 016 193	1 620 501
40	21	41	7 164	22 453	927 478	1 964 606	4 147 802
45	23	46	10 162	31 763	1 669 854	3 517 049	9 489 198
50	26	51	13 955	43 400	2 826 857	5 924 678	19 889 522
55	28	56	18 532	57 521	4 550 607	9 500 348	38 823 982
60	31	61	24 079	74 480	7 029 519	14 625 206	71 488 151
65	33	66	30 568	94 413	10 486 290	21 755 660	125 315 638
70	36	71	38 204	117 693	15 187 768	31 429 928	210 705 824
75	38	76	46 937	144 438	21 440 668	44 275 053	341 744 268

CaGe

Chemical and abstract Graph environment

`cone 4 5 s 8`


symmetric
nonsymmetric
Number of pentagons
4
1
5
Length of longest Side
5
isolated pentagons (ipr)
Add a number of hexagon layers
8

3e3e 6c70 6e61 7261 635f 646f 3c65 003c 016a 0002 0036 0000 0003
0001 0000 0004 0037 0002 0000 0005 0003 0000 0006 0039 0004 0000
0007 0005 0000 0008 003b 0006 0000 0009 0007 0000 000a 003d 0008
0000 000b 0009 0000 000c 003f 000a 0000 000d 000b 0000 000e 0041
000c 0000 000f 000d 0000 0010 0043 000e 0000 0011 000f 0000 0012
0045 0010 0000 0013 0011 0000 0014 0047 0012 0000 0015 0013 0000
0016 0049 0014 0000 0017 0015 0000 0018 004b 0016 0000 0019 0017
0000 001a 004d 0018 0000 001b 0019 0000 001c 004f 001a 0000 001d
001b 0000 001e 001c 0000 001f 0051 001d 0000 0020 001e 0000 0021
0052 001f 0000 0022 0020 0000 0023 0054 0021 0000 0024 0022 0000
0025 0056 0023 0000 0026 0024 0000 0027 0058 0025 0000 0028 0026
0000 0029 005a 0027 0000 002a 0028 0000 002b 005c 0029 0000 002c
002a 0000 002d 005e 002b 0000 002e 002c 0000 002f 0060 002d 0000
0030 002e 0000 0031 0062 002f 0000 0032 0030 0000 0033 0064 0031
0000 0034 0032 0000 0035 0066 0033 0000 0036 0034 0000 0001 0038
0035 0000 0003 003a 0038 0000 0037 0068 0036 0000 003c 003a 0005
0000 0039 0069 0037 0000 003e 003c 0007 0000 003b 006b 0039 0000
0040 003e 0009 0000 003d 006d 003b 0000 0042 0040 000b 0000 003f
006f 003d 0000 0044 0042 000d 0000 0041 0071 003f 0000 0046 0044

DEMO

Generation of Structures in Chemistry and Mathematics

Public Defense

Nico Van Cleemput

Combinatorial Algorithms and Algorithmic Graph Theory
Department of Applied Mathematics and Computer Science
Ghent University

UNIVERSITEIT GENT