
Counting polyhexes of size 36

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John Mason, 26 September 2023

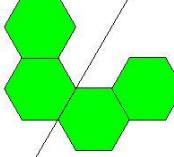
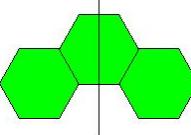
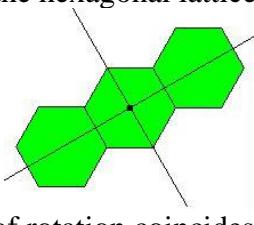
Some corrections highlighted in yellow, 27 October 2023

1 INTRODUCTION

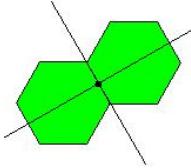
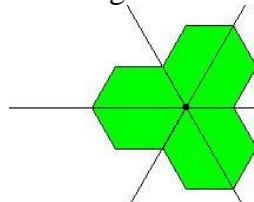
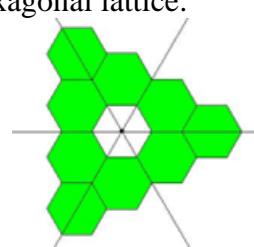
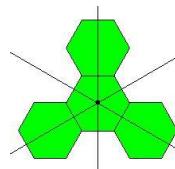
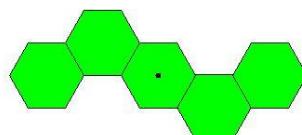
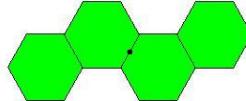
This document replaces a previous version which discussed the enumeration of polyhexes through to size 30.

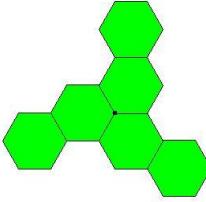
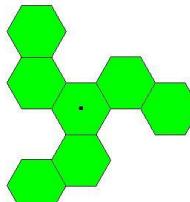
Free polyhexes¹ are enumerated by OEIS sequence A000228. In addition, A001207 enumerates the fixed polyhexes, and A006535 the one-sided.

The following table lists the possible symmetries. In each case, the symmetry X is defined to include those polyhexes satisfying said symmetry, but not those that satisfy some greater symmetry that includes X.

Acronym	Symmetry	Fixed multiplier	One-sided multiplier
ASYM	No symmetry 	12	2
MA	A single reflective symmetry, on an axis aligned to an edge of a hexagon in the underlying hexagonal lattice 	6	1
MU	A single reflective symmetry, on an axis not aligned to an edge of a hexagon in the underlying hexagonal lattice 	6	1
M2	Two reflective symmetries (one aligned, one not aligned), in axes at 90° from each other, and 180° rotational symmetry. In particular, M2C: the axis of rotation coincides with the centre of a cell of the hexagonal lattice:  or M2M: the axis of rotation coincides with the midpoint of the edge of a cell of the hexagonal lattice:	3	1

¹ [https://en.wikipedia.org/wiki/Polyhex_\(mathematics\)](https://en.wikipedia.org/wiki/Polyhex_(mathematics))

			
M3A	<p>Three reflective symmetries, on axes aligned to edges, at 60° from each other, and 120° rotational symmetry.</p> <p>In particular, M3AV: the axis of rotation coincides with a vertex of a cell of the hexagonal lattice:</p>  <p>or M3AC: the axis of rotation coincides with the centre of a cell of the hexagonal lattice:</p> 	2	1
M3U	<p>Three reflective symmetries, on axes not aligned to edges, at 60° from each other, and 120° rotational symmetry</p> 	2	1
R180	<p>180° rotational symmetry.</p> <p>In particular, R180C: the axis of rotation coincides with the centre of a cell of the hexagonal lattice:</p>  <p>or R180M: the axis of rotation coincides with the midpoint of the edge of a cell of the hexagonal lattice:</p> 	6	2
R120	<p>120° rotational symmetry.</p> <p>In particular, R120V: the axis of rotation coincides with a vertex of a cell of the hexagonal lattice:</p>	4	2

	 <p>or R120C: the axis of rotation coincides with the centre of a cell of the hexagonal lattice:</p> 		
R60	60° rotational symmetry	2	2
ALL	With all symmetries (reflective symmetry in 6 axes, 60° rotational symmetry, consequent 120° and 180° rotational symmetries)	1	1

Therefore, two simple formulae may be stated.

Formula 1:

$$\text{Free}(n) = \text{ASYM}(n) + \text{MA}(n) + \text{MU}(n) + \text{M2C}(n) + \text{M2M}(n) + \text{M3AV}(n) + \text{M3AC}(n) + \text{M3U}(n) + \text{R120C}(n) + \text{R120V}(n) + \text{R180M}(n) + \text{R180C}(n) + \text{R60}(n) + \text{ALL}(n)$$

Formula 2:

$$\text{Fixed}(n) = 12 * \text{ASYM}(n) + 6 * \text{MA}(n) + 6 * \text{MU}(n) + 3 * \text{M2C}(n) + 3 * \text{M2M}(n) + 2 * \text{M3AV}(n) + 2 * \text{M3AC}(n) + 2 * \text{M3U}(n) + 4 * \text{R120C}(n) + 4 * \text{R120V}(n) + 6 * \text{R180M}(n) + 6 * \text{R180C}(n) + 2 * \text{R60}(n) + \text{ALL}(n)$$

As a consequence, eliminating ASYM(n), we have

Formula 3:

$$\begin{aligned} \text{Free}(n) = & (6 * \text{MA}(n) + 6 * \text{MU}(n) + 9 * \text{M2C}(n) + 9 * \text{M2M}(n) + 10 * \text{M3AV}(n) + 10 * \text{M3AC}(n) \\ & + 10 * \text{M3U}(n) + 8 * \text{R120C}(n) + 8 * \text{R120V}(n) + 6 * \text{R180M}(n) + 6 * \text{R180C}(n) + 10 * \text{R60}(n) \\ & + 11 * \text{ALL}(n) + \text{Fixed}(n)) / 12 \end{aligned}$$

As of July 2023, the principal sequences had been published through to the following maximum indexes:

Sequence	Content	n
A000228	Free	21
A001207	Fixed	46
A006535	One-sided	20
A030225	Achiral	36
A030226	Chiral	20

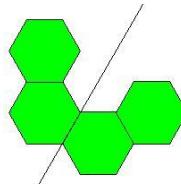
In order to calculate Free (21) through Free (36) using Formula 3, it is necessary to enumerate each specific symmetry through to size 36.

The enumeration was programmed according to the basic principles outlined in Redelmeier's paper² to which reference should be made for a more complete explanation:

1. From the starting cell, choose an adjacent hexagon. Then explore recursively the two possible forks: (i) that hexagon is occupied, and (ii) that hexagon is not occupied. This method will generally count fixed polyhexes.
2. For polyhexes with rotational symmetry, use inner rings as detailed below.

Method 1 was used for polyhexes with mirror symmetry. In particular, 3 programs were developed:

- MU symmetry
- MA symmetry for polyhexes having no cell bisected by the axis of symmetry



- MA symmetry for polyhexes having at least one cell bisected by the axis of symmetry³



² [Counting Polyominoes: yet another attack. D. Hugh Redelmeier 1980](#)

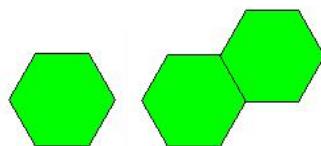
³ Russell makes a similar distinction: see <https://oeis.org/A030225>

Polyhexes with rotational symmetry were enumerated using Method 2. Non-trivial inner rings with rotational symmetry were identified as per the following table:

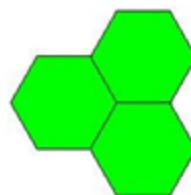
Size/Sym	ALL	R60	R180C	R180M	R120V	R120C	M3U	M3AC	M3AV	M2M	M2C
3	0	0	0	0	0	0	0	0	1	0	0
4	0	0	0	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0	0	0	0	0
6	1	0	0	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0	0	0	1	0
9	0	0	0	0	0	0	0	0	1	0	0
10	0	0	0	0	0	0	0	0	0	1	1
11	0	0	0	0	0	0	0	0	0	0	0
12	1	0	0	2	0	0	1	0	1	1	1
13	0	0	0	0	0	0	0	0	0	0	0
14	0	0	1	4	0	0	0	0	0	3	3
15	0	0	0	0	2	0	0	1	1	0	0
16	0	0	4	14	0	0	0	0	0	4	3
17	0	0	0	0	0	0	0	0	0	0	0
18	2	0	11	37	3	1	3	0	2	7	8
19	0	0	0	0	0	0	0	0	0	0	0
20	0	0	34	103	0	0	0	0	0	10	10
21	0	0	0	0	11	4	0	1	4	0	0
22	0	0	91	272	0	0	0	0	0	23	23
23	0	0	0	0	0	0	0	0	0	0	0
24	2	1	257	735	24	10	9	2	6	27	23
25	0	0	0	0	0	0	0	0	0	0	0
26	0	0	672	1957	0	0	0	0	0	56	69
27	0	0	0	0	74	30	0	5	8	0	0
28	0	0	1839	5228	0	0	0	0	0	73	69
29	0	0	0	0	0	0	0	0	0	0	0
30	5	2	4873	13955	174	84	24	5	15	167	166
31	0	0	0	0	0	0	0	0	0	0	0
32	0	0	13127	37371	0	0	0	0	0	192	187
33	0	0	0	0	489	222	0	10	25	0	0
34	0	0	35001	100178	0	0	0	0	0	431	486
35	0	0	0	0	0	0	0	0	0	0	0
36	5	8	94177	269126	1218	606	68	17	42	528	499
37	0	0	0	0	0	0	0	0	0	0	0
38	0	0	252597	724310	0	0	0	0	0	1219	1268
39	0	0	0	0	3332	1572	0	33	59	0	0
40	0	0	680710	1953195	0	0	0	0	0	1415	1382

In the previous version of this document, rings had been identified only up to size 30, and this created the bottleneck that impeded polyhex enumeration beyond that size. The ring generating algorithm produced rings of all symmetries, including asymmetrical ones: at size 30, there are 50K symmetrical rings and 76 million asymmetric rings. Robert A. Russell gave a new algorithm for generating rings of each specific rotational symmetry, allowing the identification of size 40 rings in reasonable time.

The following trivial rings (labelled T1, T2) are also needed:



In a previous version of this document, T3 (see below) was also described as a trivial ring whereas it satisfies the criteria of being a ring (each cell touches precisely 2 other cells) without any problem.



This table shows which rings are needed for each rotational symmetry:

Symmetry	Required rings					
ALL	T1	ALL				
R60	T1	ALL	R60			
R180C	T1	ALL	R60	M2C	R180C	
R180M	T2	M2M	R180M			
R120V	M3AV	R120V				
R120C	T1	ALL	R60	M3U	M3AC	R120C

Both R60 and ALL symmetries are enumerated by other programs and so were not specifically implemented.

This table shows the outputs of each program (which in the case of the rotational symmetries, correspond to the input rings).

Program	Outputs					
R180C	ALL	R60	M2C	R180C		
R180M	M2M	R180M				
R120V	M3AV	R120V				
R120C	ALL	R60	M3U	M3AC	R120C	
MA⁴	ALL	M3AC	M3AV	M2M	M2C	MA
MU	ALL	M3U	M2M	M2C	MU	

⁴ Separate programs for “with” or “without” at least one cell bisected by the axis of symmetry

As discussed by Redelmeier, the algorithm for enumerating polyforms with rotational symmetry consists of identifying the inner rings, and then performing internal and external growth. The condition of performing internal growth is that any polyform generated from one specific inner ring must not have a more “internal” inner ring. For polyhexes, this was implemented as follows:

- a. Identify the distinct islands that the inner growth has produced.
- b. No island may touch more than 2 hexagons of the inner ring; if an island does touch 2 hexagons of the inner ring, these must be adjacent.

2 INTERMEDIATE RESULTS

The following tables show the results of each program.

R180C

Size	ALL	R60	R180C	M2C
1	1	0	0	0
2	0	0	0	0
3	0	0	0	1
4	0	0	0	0
5	0	0	1	2
6	1	0	0	0
7	1	0	7	3
8	0	0	0	2
9	0	0	36	7
10	0	0	3	5
11	0	0	177	15
12	3	0	24	9
13	2	0	862	28
14	0	0	136	27
15	0	0	4182	62
16	0	0	733	63
17	0	0	20375	128
18	5	3	3820	137
19	2	2	99733	268
20	0	0	19590	329
21	0	0	490490	565
22	0	0	99842	734
23	0	0	2422546	1203
24	13	15	507332	1678
25	4	8	12010068	2541
26	0	0	2575438	3754
27	0	0	59736164	5455
28	0	0	13071230	8638
29	0	0	297964711	11641
30	28	77	66357160	19104
31	8	33	1489953995	25088
32	0	0	337008950	43937
33	0	0	7466755274	53880
34	0	0	1712458699	97226
35	0	0	37491550356	116699
36	63	363	8706384438	222953

R180M

Size	R180M	M2M
1	0	0
2	0	1
3	0	0
4	1	2
5	0	0
6	7	3
7	0	0
8	35	7
9	0	0
10	172	14
11	0	0
12	833	31
13	0	0
14	4044	64
15	0	0
16	19698	145
17	0	0
18	96464	303
19	0	0
20	474607	683
21	0	0
22	2345344	1448
23	0	0
24	11633557	3273
25	0	0
26	57896017	6994
27	0	0
28	288948867	15815
29	0	0
30	1445685446	34016
31	0	0
32	7248934739	76974
33	0	0
34	36417693505	166368
35	0	0
36	183271927110	376726

R120V

Size	R120V	M3AV
1	0	0
2	0	0
3	0	1
4	0	0
5	0	0
6	1	1
7	0	0
8	0	0
9	5	2
10	0	0
11	0	0
12	23	5
13	0	0
14	0	0
15	109	9
16	0	0
17	0	0
18	507	19
19	0	0
20	0	0
21	2377	39
22	0	0
23	0	0
24	11232	82
25	0	0
26	0	0
27	53509	171
28	0	0
29	0	0
30	256820	368
31	0	0
32	0	0
33	1240714	773
34	0	0
35	0	0
36	6027760	1678

R120C

Size	ALL	R60	R120C	M3U	M3AC
1	1	0	0	0	0
2	0	0	0	0	0
3	0	0	0	0	0
4	0	0	0	1	0
5	0	0	0	0	0
6	1	0	0	0	0
7	1	0	1	1	0
8	0	0	0	0	0
9	0	0	0	1	1
10	0	0	5	3	1
11	0	0	0	0	0
12	3	0	3	2	0
13	2	0	26	5	0
14	0	0	0	0	0
15	0	0	17	7	3
16	0	0	120	12	2
17	0	0	0	0	0
18	5	3	90	17	5
19	2	2	556	24	3
20	0	0	0	0	0
21	0	0	466	42	15
22	0	0	2589	53	7
23	0	0	0	0	0
24	13	15	2302	100	27
25	4	8	12134	108	11
26	0	0	0	0	0
27	0	0	11352	230	69
28	0	0	57360	235	26
29	0	0	0	0	0
30	28	77	55597	557	140
31	8	33	273238	496	46
32	0	0	0	0	0
33	0	0	273125	1237	324
34	0	0	1310951	1072	98
35	0	0	0	0	0
36	63	363	1343539	2973	689

MA{COA} (MA: At least one cell on axis of symmetry)

Size	ALL	M3AC	M3AV	M2M	M2C	MA
1	1	0	0	0	0	0
2	0	0	0	0	0	0
3	0	0	1	0	1	0
4	0	0	0	1	0	0
5	0	0	0	0	2	4
6	0	0	1	1	0	1
7	1	0	0	0	3	18
8	0	0	0	4	1	9
9	0	1	2	0	7	78
10	0	1	0	6	1	49
11	0	0	0	0	15	363
12	2	0	4	18	5	233
13	2	0	0	0	28	1652
14	0	0	0	30	9	1155
15	0	3	9	0	62	7596
16	0	2	0	87	38	5506
17	0	0	0	0	128	35442
18	2	4	16	153	55	26474
19	2	3	0	0	268	166740
20	0	0	0	419	204	127465
21	0	15	39	0	565	791106
22	0	7	0	764	331	616475
23	0	0	0	0	1203	3781081
24	9	21	68	2045	1061	2991732
25	4	11	0	0	2541	18182439
26	0	0	0	3818	1820	14578029
27	0	69	171	0	5455	87902062
28	0	26	0	10029	5553	71272778
29	0	0	0	0	11641	426928553
30	16	112	309	19061	9761	349575126
31	8	46	0	0	25088	2081932918
32	0	0	0	49413	28614	1719460611
33	0	324	773	0	53880	10188911027
34	0	98	0	95211	51677	8479568368
35	0	0	0	0	116699	50022521369
36	45	554	1415	244351	146787	41915714380

MA{NCOA} (MA: No cell on axis of symmetry)

Size	ALL	M3AC	M3AV	M2M	M2C	MA
1	0	0	0	0	0	0
2	0	0	0	1	0	0
3	0	0	0	0	0	0
4	0	0	0	1	0	1
5	0	0	0	0	0	0
6	1	0	0	2	0	4
7	0	0	0	0	0	0
8	0	0	0	3	1	20
9	0	0	0	0	0	0
10	0	0	0	8	4	87
11	0	0	0	0	0	0
12	1	0	1	13	4	397
13	0	0	0	0	0	0
14	0	0	0	34	18	1800
15	0	0	0	0	0	0
16	0	0	0	58	25	8303
17	0	0	0	0	0	0
18	3	1	3	150	82	38558
19	0	0	0	0	0	0
20	0	0	0	264	125	181141
21	0	0	0	0	0	0
22	0	0	0	684	403	857473
23	0	0	0	0	0	0
24	4	6	14	1228	617	4090162
25	0	0	0	0	0	0
26	0	0	0	3176	1934	19630988
27	0	0	0	0	0	0
28	0	0	0	5786	3085	94741962
29	0	0	0	0	0	0
30	12	28	59	14955	9343	459406445
31	0	0	0	0	0	0
32	0	0	0	27561	15323	2237018980
33	0	0	0	0	0	0
34	0	0	0	71157	45549	10933018521
35	0	0	0	0	0	0
36	18	135	263	132375	76166	53608544811

Correction (27 October 2023): The following formula applies, similar to one used in the calculation of [A349329](#):

$$\text{MA}\{\text{NCOA}\}(n) = 6*\text{ASYM}(n/2) + 3*\text{MA}(n/2) + 2*\text{MU}(n/2) + \text{M2}(n/2) + \text{MA}(n/2) + 3*\text{R180}(n/2) + 2*\text{R120}(n/2) + \text{R60}(n/2) - \text{M3A}\{\text{NCOA}\}(n) \text{ (where R180}(k) = \text{R180C}(k) + \text{R180M}(k), \text{etc.)}$$

Remember that the results in this table are only partial; for example, the correct value for M2M(n) requires the sum of the corresponding values in this table (no cell on axis) and the previous one (at least one cell on axis).

MA (Totals)

Size	ALL	M3AC	M3AV	M2M	M2C	MA
1	1	0	0	0	0	0
2	0	0	0	1	0	0
3	0	0	1	0	1	0
4	0	0	0	2	0	1
5	0	0	0	0	2	4
6	1	0	1	3	0	5
7	1	0	0	0	3	18
8	0	0	0	7	2	29
9	0	1	2	0	7	78
10	0	1	0	14	5	136
11	0	0	0	0	15	363
12	3	0	5	31	9	630
13	2	0	0	0	28	1652
14	0	0	0	64	27	2955
15	0	3	9	0	62	7596
16	0	2	0	145	63	13809
17	0	0	0	0	128	35442
18	5	5	19	303	137	65032
19	2	3	0	0	268	166740
20	0	0	0	683	329	308606
21	0	15	39	0	565	791106
22	0	7	0	1448	734	1473948
23	0	0	0	0	1203	3781081
24	13	27	82	3273	1678	7081894
25	4	11	0	0	2541	18182439
26	0	0	0	6994	3754	34209017
27	0	69	171	0	5455	87902062
28	0	26	0	15815	8638	166014740
29	0	0	0	0	11641	426928553
30	28	140	368	34016	19104	808981571
31	8	46	0	0	25088	2081932918
32	0	0	0	76974	43937	3956479591
33	0	324	773	0	53880	10188911027
34	0	98	0	166368	97226	19412586889
35	0	0	0	0	116699	50022521369
36	63	689	1678	376726	222953	95524259191

MU

Size	ALL	M3U	M2M	M2C	MU
1	1	0	0	0	0
2	0	0	1	0	0
3	0	0	0	1	1
4	0	1	2	0	0
5	0	0	0	2	5
6	1	0	3	0	7
7	1	1	0	3	23
8	0	0	7	2	37
9	0	1	0	7	113
10	0	3	14	5	182
11	0	0	0	15	536
12	3	2	31	9	901
13	2	5	0	28	2535
14	0	0	64	27	4390
15	0	7	0	62	12117
16	0	12	145	63	21326
17	0	0	0	128	58289
18	5	17	303	137	104040
19	2	24	0	268	282002
20	0	0	683	329	509175
21	0	42	0	565	1372060
22	0	53	1448	734	2500446
23	0	0	0	1203	6707057
24	13	100	3273	1678	12319637
25	4	108	0	2541	32918368
26	0	0	6994	3754	60879348
27	0	230	0	5455	162132815
28	0	235	15815	8638	301639803
29	0	0	0	11641	801000925
30	28	557	34016	19104	1498093162
31	8	496	0	25088	3967928016
32	0	0	76974	43937	7456094865
33	0	1237	0	53880	19702946335
34	0	1072	166368	97226	37180432500
35	0	0	0	116699	98044669731
36	63	2973	376726	222953	185724075649

3 FINAL RESULTS

Summary of symmetry enumeration

Size	MA	MU	M2C	M2M	M3AC	M3AV	M3U	R120C	R120V	R180M	R180C	R60	ALL
1	0	0	0	0	0	0	0	0	0	0	0	0	1
2	0	0	0	1	0	0	0	0	0	0	0	0	0
3	0	1	1	0	0	1	0	0	0	0	0	0	0
4	1	0	0	2	0	0	1	0	0	1	0	0	0
5	4	5	2	0	0	0	0	0	0	0	1	0	0
6	5	7	0	3	0	1	0	0	1	7	0	0	1
7	18	23	3	0	0	0	1	1	0	0	7	0	1
8	29	37	2	7	0	0	0	0	0	35	0	0	0
9	78	113	7	0	1	2	1	0	5	0	36	0	0
10	136	182	5	14	1	0	3	5	0	172	3	0	0
11	363	536	15	0	0	0	0	0	0	0	177	0	0
12	630	901	9	31	0	5	2	3	23	833	24	0	3
13	1652	2535	28	0	0	0	5	26	0	0	862	0	2
14	2955	4390	27	64	0	0	0	0	0	4044	136	0	0
15	7596	12117	62	0	3	9	7	17	109	0	4182	0	0
16	13809	21326	63	145	2	0	12	120	0	19698	733	0	0
17	35442	58289	128	0	0	0	0	0	0	0	20375	0	0
18	65032	104040	137	303	5	19	17	90	507	96464	3820	3	5
19	166740	282002	268	0	3	0	24	556	0	0	99733	2	2
20	308606	509175	329	683	0	0	0	0	0	474607	19590	0	0
21	791106	1372060	565	0	15	39	42	466	2377	0	490490	0	0
22	1473948	2500446	734	1448	7	0	53	2589	0	2345344	99842	0	0
23	3781081	6707057	1203	0	0	0	0	0	0	0	2422546	0	0
24	7081894	12319637	1678	3273	27	82	100	2302	11232	11633557	507332	15	13
25	18182439	32918368	2541	0	11	0	108	12134	0	0	12010068	8	4
26	34209017	60879348	3754	6994	0	0	0	0	0	57896017	2575438	0	0
27	87902062	162132815	5455	0	69	171	230	11352	53509	0	59736164	0	0
28	166014740	301639803	8638	15815	26	0	235	57360	0	288948867	13071230	0	0
29	426928553	801000925	11641	0	0	0	0	0	0	0	297964711	0	0
30	808981571	1498093162	19104	34016	140	368	557	55597	256820	1445685446	66357160	77	28
31	2081932918	3967928016	25088	0	46	0	496	273238	0	0	1489953995	33	8
32	3956479591	7456094865	43937	76974	0	0	0	0	0	7248934739	337008950	0	0
33	10188911027	19702946335	53880	0	324	773	1237	273125	1240714	0	7466755274	0	0
34	19412586889	37180432500	97226	166368	98	0	1072	1310951	0	36417693505	1712458699	0	0
35	50022521369	98044669731	116699	0	0	0	0	0	0	0	37491550356	0	0
36	95524259191	185724075649	222953	376726	689	1678	2973	1343539	6027760	183271927110	8706384438	363	63

Each of these columns is a potential OEIS sequence. If they are published, it must be decided whether or not to aggregate, for example, R180M and R180C. In the case of polyominoes, sequences exist for both the aggregated and non-aggregated symmetries.

OEIS sequences. New values (calculated since July 2023) are shown in bold.

Size	A000228 Free	A006535 One-sided	A030225 Achiral	A030226 Chiral	A364306 Asym
1	1	1	1	0	0
2	1	1	1	0	0
3	3	3	3	0	0
4	7	10	4	3	2
5	22	33	11	11	10
6	82	147	17	65	57
7	333	620	46	287	279
8	1448	2821	75	1373	1338
9	6572	12942	202	6370	6329
10	30490	60639	341	30149	29969
11	143552	286190	914	142638	142461
12	683101	1364621	1581	681520	680637
13	3274826	6545430	4222	3270604	3269716
14	15796897	31586358	7436	15789461	15785281
15	76581875	153143956	19794	76562081	76557773
16	372868101	745700845	35357	372832744	372812193
17	1822236628	3644379397	93859	1822142769	1822122394
18	8934910362	17869651166	169558	8934740804	8934639920
19	43939164263	87877879487	449039	43938715224	43938614933
20	216651036012	433301253231	818793	216650217219	216649723022
21	1070793308942	2141584454057	2163827	1070791145115	1070790651782
22	5303855973849	10607707971062	3976636	5303851997213	5303849549438
23	26323064063884	52646117638427	10489341	26323053574543	26323051151997
24	130878392115834	261756764824964	19406704	130878372709130	130878360554692
25	651812979669234	1303625908234997	51103471	651812928565763	651812916543553
26	3251215493161062	6502430891223011	95099113	3251215398061949	3251215337590494
27	16240020734253127	32480041218465452	250040802	16240020484212325	16240020424411300
28	81227147768301723	162454295068924189	467679257	81227147300622466	81227146998545009
29	406770970805865187	813541940383789255	1227941119	406770969577924068	406770969279959357
30	2039375198751047333	4078750395194965720	2307128946	2039375196443918387	2039375194931563287
31	10235534401150791938	20471068796251697304	6049886572	2039375196443918387	10235534393610678100
32	51423416130016135698	102846832248619576029	11412695367	10235534395100905366	51423416111017496642
33	258596002056308380673	517192004082724847770	29891913576	51423416118603440331	258596002018948197984
34	1301574358659039221669	2603148717261485159185	56593284153	258596002026416467097	1301574358564314474361
35	6556625094801580406231	13113250189455093504663	148067307799	1301574358602445937516	6556625094616021548076
36	33054884840256184854480	66109769680231120769038	281248939922	6556625094653513098432	33054884839782950231348

4 CONCLUSIONS

The approach is heavily dependent the calculation of Fixed(n).

The level of confidence in the results depends mainly on the following factors:

1. Consistency with existing enumerations of free and one-sided polyhexes.
2. Consistency with Russell's enumeration of achiral polyhexes.
3. Redundancy of outputs of different programs. For example, the values for M2C(n) were generated by 3 different programs (MA, MU, R180C) all with the same outcome. The implementation of R180C, based on inner rings, is significantly different to the implementation of programs based on mirror symmetry.
4. The built-in check of Formula 3. If the sum (see note⁵) is not a multiple of 12, the calculation is wrong.

The following are the most important runtimes:

1. R180C about 30 hours
2. R180M about 15 hours
3. MU about 8 hours
4. MA (COA) about 20 hours
5. MA (NCOA) about 30 hours

⁵ $(6*MA(n) + 6*MU(n) + 9*M2C(n) + 9*M2M(n) + 10*M3AV(n) + 10*M3AC(n) + 10*M3U(n) + 8*R120C(n) + 8*R120V(n) + 6*R180M(n) + 6*R180C(n) + 10*R60(n) + ALL(n) + Fixed(n))$

Alternative calculation

Recalling Formula 3:

$$\begin{aligned} \text{Free}(n) = & (6*\text{MA}(n)+6*\text{MU}(n)+9*\text{M2C}(n)+9*\text{M2M}(n)+10*\text{M3AV}(n)+10*\text{M3AC}(n) \\ & +10*\text{M3U}(n)+8*\text{R120C}(n)+8*\text{R120V}(n)+6*\text{R180M}(n)+6*\text{R180C}(n)+10*\text{R60}(n) \\ & +11*\text{ALL}(n) \\ & +\text{Fixed}(n))/12 \end{aligned}$$

Formula 4:

$$\text{Achiral}(n) = \text{MA}(n)+\text{MU}(n)+\text{M2C}(n)+\text{M2M}(n)+\text{M3AV}(n)+\text{M3AC}(n)+\text{M3U}(n)+\text{ALL}(n)$$

Hence:

$$\text{MA}(n)+\text{MU}(n) = \text{Achiral}(n)-\text{M2C}(n)-\text{M2M}(n)-\text{M3AV}(n)-\text{M3AC}(n)-\text{M3U}(n)-\text{ALL}(n)$$

We can therefore deduce Formula 5:

$$\begin{aligned} \text{Free}(n) = & (6*\text{Achiral}(n)+3*\text{M2C}(n)+3*\text{M2M}(n)+4*\text{M3AV}(n)+4*\text{M3AC}(n) \\ & +4*\text{M3U}(n)+8*\text{R120C}(n)+8*\text{R120V}(n)+6*\text{R180M}(n)+6*\text{R180C}(n)+10*\text{R60}(n)+5*\text{ALL}(n) \\ & +\text{Fixed}(n))/12 \end{aligned}$$

In this way, $\text{Free}(n)$ can be calculated using fewer CPU-hours, if $\text{Achiral}(n)$ is available. On the other hand, in this way we lose one of the useful factors of verification.

For any further information, or to point out errors, please contact me at this email address:
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