Correction of A036672(10) and A036673(10)

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The sequence A036672 [2] counts the total number of stereo-isomers of acyclic hydrocarbons with a given number of carbon atoms. Similarly, A036673 [3] is total excluding hydrocarbons containing triple bonds. Theory and tables of numbers for counting these compounds was developed by Ronald C. Read and published in [4], in particular §7, pp. 53–61.

It was found the values given for A036672(10) and A036673(10) by Read are incorrect, most likely due to a numerical error during computation. We give corrected values.

The starting point for these calculations is the trivariate generating function defined by

$$g(x,y,z) = 1+x\left\{\frac{1}{3}\left[g^3(x,y,z)+2g(x^3,y^3,z^3)\right]+\frac{xy}{1-xy}g^3(x,y,z)+xzg(x,y,z)\right\}.$$

The coefficient $[x^n y^d z^t]g(x,y,z)$ is the number of stereo-isomers of mono-valent acyclic hydrocarbons with n carbon atoms, d double bonds, t triple bonds, and one labelled atom. Table V on p. 55 of [4] gives these coefficients for $n \le 11$. This table is correct.

Using $g(x,y,z)$ and $g_1(x,y,z) = g(x,y,z)-1$, Read derives the following contributions to the total number of acylic stereo-isomers (equation numbering following Read):

$$l(x,y,z) =$$

$$xZ(A_4; g(x,y,z)) + x^2 z g^2(x,y,z) \tag{7.6}$$

$$+\frac{1}{2}\frac{x^2y}{(1-x^2y^2)^2}\left[g^4(x,y,z)+g^2(x^2,y^2,z^2)\right] \tag{7.8}$$

$$+\frac{1}{2}\frac{x^3y^2}{(1-x^2y^2)^2}\left[g^4(x,y,z)+g^2(x^2,y^2,z^2)\right] \tag{7.9}$$

$$+\frac{1}{4}\frac{x^3y^2}{1-x^2y^2}\left[g^4(x,y,z)+3g^2(x^2,y^2,z^2)\right] \tag{7.10}$$

$$-\frac{1}{2}\left[g_1^2(x,y,z)-g_1(x^2,y^2,z^2)\right] \tag{7.11}$$

$$-\frac{1}{2}x^2z\left[g^2(x,y,z)-g(x^2,y^2,z^2)\right] \tag{7.12}$$

$$-\frac{1}{2}\frac{x^3y^2}{(1-x^2y^2)^2}\left[g^4(x,y,z)+g^2(x^2,y^2,z^2)\right] \tag{7.13}$$

$$-\frac{1}{2}\frac{x^4y^3}{(1-x^2y^2)^2}\left[g^4(x,y,z)+g^2(x^2,y^2,z^2)\right] \tag{7.14}$$

$$-\frac{1}{4}\frac{x^2y}{1-x^2y^2}\left[g^4(x,y,z)+3g^2(x^2,y^2,z^2)\right] \tag{7.15}$$

$$+\frac{x^2y}{1-x^2y^2}g^2(x^2,y^2,z^2). \tag{7.16}$$

Equations (7.12) and (7.13) are not actually numbered in Read although they are referred to. In Read, (7.15) mistakenly has $3g^3$ rather than $3g^2$. As noted by Read, (7.13) cancels with (7.9). Read offers a simplification of this large expression at the bottom of page 59, but it appears to be incorrect.

The above expression was implemented in Java within the jOEIS [1] project and the terms of A036672 and A036673 computed. Our values appear at the end on this note. It was discovered that the computed values did not match the existing values for $n = 10$. After investigation, the mostly likely explanation is a numerical error in the original computation.

A table of the corresponding coefficients of $l(x, y, z)$ for $n \leq 10$ appears in Table VI of Read. The section of this table for $n = 10$ along with a corrected version is:

	t					
	0	1	2	3	4	5
0	136	338	325	135	23	1
1	895	1717	1102	238	11	
2	2418	3214	1164	86		
3	3356	2720	443	5		
4	5784	1108	60			
d 5	1135	223	4			
6	295	23				
7	52	1				
8	87					
9	11					

Read, p. 60

	t					
	0	1	2	3	4	5
0	136	338	325	135	23	1
1	895	1717	1102	238	11	
2	2418	3214	1164	86		
3	3356	2720	443	5		
4	**2557**	1108	60			
d 5	1135	223	4			
6	295	23				
7	52	1				
8	**5**					
9	**1**					

Corrected

A036672(10) corresponds to the sum of the numbers in this table, whereas A036673(10) is the sum of the numbers in the column $t = 0$.

The error $[x^{10}y^9z^0]l(x, y, z) = 11$ is typographical, since Read already computes the sum as 27100 (rather than 27110) and it is obvious that there is only one stereoisomer with 9 double bonds. The other two errors are harder to explain, but possibly a mistake was made in the computation of (7.14). That $[x^{10}y^8z^0]l(x, y, z) = 5$ is readily seen by noting the required hydrocarbons are:

```
C=C=C=C=C=C=C=C=C-C
C=C=C=C=C=C=C=C-C=C
C=C=C=C=C=C=C-C=C=C
C=C=C=C=C=C-C=C=C=C
C=C=C=C=C-C=C=C=C=C
```

n	A036672(n)	A036673(n)
2	1	1
3	3	2
4	4	3
5	13	9
6	31	20
7	109	64
8	372	205
9	1446	747
10	5714	2767
11	23791	10850
12	100827	43254
13	438019	176990
14	1931818	735007
15	8648820	3099272
16	39178079	13220407
17	179383748	57001841
18	828905252	248009246
19	3861958783	1087947441
20	18125392905	4807232915
21	85631735301	21381055533
22	406977645228	95660032110
23	1944737525915	430298114499
24	9338989516911	1945096434552
25	45051405221284	8832200860663
26	218236995129380	40271358004756
27	1061256971559421	184325394540531
28	5179178238707032	846667179332120
29	25359378786128904	3901838533839904
30	124553113387147741	18036676275203557

References

[1] Sean A. Irvine. jOEIS. `https://github.com/archmageirvine/joeis`, 2020.

[2] OEIS Foundation Inc. A036672, the on-line encyclopedia of integer sequences. `http://oeis.org/A036672`, 2020.

[3] OEIS Foundation Inc. A036773, the on-line encyclopedia of integer sequences. `http://oeis.org/A036673`, 2020.

[4] Ronald C. Read. The enumeration of acyclic chemical compounts. In Alexandru T. Balaban, editor, *Chemical Applications of Graph Theory*. Academic Press, London, 1976.