An algebraic solution for the numbers of staggered conformers of alkanes ☆

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The staggered conformers of alkanes are counted by using a tree-counting method. Some numerical results are tabulated.

The algebraic solution for the numbers of staggered conformers of alkanes can be found by using a tree-counting method, which is similar to that used for the enumeration of configurations of alkanes and other acyclic compounds [1–4]. Each conformer enantiomer pair is counted double.

Let $a(x)$ be the generating function for counting staggered conformers of alkyls. Let $c(x)$ be the generating function for counting staggered conformers of alkyls with C_3 symmetry. Let $d(x)$ be the generating function for counting staggered conformers of alkyls without C_3 symmetry. So we have

$$a(x) = d(x) + c(x)\,. \tag{1}$$

When an alkyl without C_3 symmetry is connected to another alkyl without C_3 symmetry, there arise three conformers. Otherwise there is just one conformer. Let $b(x)$ be the generating function of the space positions of conformers of alkyls related to another alkyl without C_3 symmetry. Then

$$b(x) = 3d(x) + c(x)\,. \tag{2}$$

Thus we establish the following recurrence formula:

$$a(x) = \sum_{i=0}^{\infty} a_i x^i = 1 + \tfrac{1}{3}x[b^3(x) + 2b(x^3)]\,, \tag{3}$$

$$c(x) = \sum_{i=0}^{\infty} c_i x^i = 1 + x \cdot b(x^3)\,. \tag{4}$$

☆ The solution of the open problem in J. Math. Chem. 17 (1995), see ref. [5].

Table 1
The numbers of conformers of alkyls and alkanes.

i	a_i	b_i	c_i	d_i	e_i
0	1	1	1	0	
1	1	1	1	0	1
2	1	3	0	1	1
3	4	12	0	4	1
4	19	55	1	18	4
5	91	273	0	91	10
6	476	1428	0	476	40
7	2586	7752	3	2583	171
8	14421	43263	0	14421	831
9	82225	246675	0	82225	4147
10	476913	1430715	12	476901	21822
11	2804880	8414640	0	2804880	117062
12	16689036	50067108	0	16689036	642600
13	100276894	300830572	55	100276839	3582322
14	607588840	1822766520	0	607588840	20256885

Here the a_i is the number of all staggered conformers of alkyls containing i carbon atoms and the c_i is the number of staggered conformers of alkyls with C_3 symmetry. We have $a_0 = 1, b_0 = 1, c_0 = 1$. Some results are given in Table 1.

Let $e(x)$ be the generating function for counting staggered conformers of alkanes. Using the same method as for the enumeration of configurations of alkanes, we obtain

$$\begin{aligned} e(x) = \sum_{i=0}^{\infty} e_i x^i = \tfrac{1}{12}x[b^4(x) + 3b^2(x^2) + 8b(x)b(x^3)] \\ - b(x)[c(x) - 1] + a(x) \cdot [c(x) - 1] \\ - \tfrac{1}{2}\{3d^2(x) + 2d(x)[c(x) - 1] \\ + [c(x) - 1]^2 - b(x^2) + 1\}\,. \end{aligned} \tag{5}$$

Here e_i is the number of all staggered conformers of alkanes containing i carbon atoms. Some results are given in Table 1.

References

[1] R.W. Robinson, F. Harary and A.T. Balaban, Tetrahedron 32 (1976) 355.
[2] J. Wang and Q. Wang, Tetrahedron 47 (1991) 2969.
[3] J. Wang and F. Gu, J. Chem. Inform. Comput. Sci. 31 (1991) 552.
[4] F. Gu and J. Wang, J. Chem. Inform. Comput. Sci. 32 (1992) 407.
[5] S.J. Cyvin, J. Math. Chem. 17 (1995) 292.