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THE NUMBERS OF CONSTITUTIONS, CONFIGURATIONS, CHIRAL AND ACHIRAL CONFIGURATIONS OF POLYHALOALKANES $C_iH_{2i+2-j}X_j$

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Abstract In this paper, we present three recurrence formulae for counting constitutions, configurations and achiral configurations of "polyhaloalkyls", $C_iH_{2i+1-j}X_j$ (j=0 — 2i+1), for the first time; and obtain a generating function for counting chiral configurations of "polyhaloalkyls", $C_iH_{2i+1-j}X_j$, and four generating functions for counting constitutions, configurations, achiral and chiral configurations of "polyhaloalkanes", $C_iH_{2i+2-j}X_j$ (j=0 — 2i+2). The numerical results are tabulated.

The enumerations of constitutions, configurations, chiral configurations and achiral configurations of alkanes have been reported[1-4]. The enumerations of isomers of some other compounds also have been reported[5-6], but the enumeration of isomers of polyhaloalkanes has not been seen.

We present three recurrence formulae for counting constitutions, configurations and achiral configurations of "polyhaloalkyls" and obtain the numbers of constitutions, configurations, chiral and achiral configurations of "polyhaloalkanes" with the graph-theoretical method[7,8].

1. DEFINITIONS

1.1 Quartic trees with two different kinds of points

Consider a tree T which consists of a finite set of two different kinds of points. A kind of points has degree 1—4, and is colored into black; another kind of points has only degree 1, and is colored into red. The number of each kind of points can be an arbitrary natural number. The tree is called a quartic tree with two different kinds of points. Quartic trees with two different kinds of points respresent constitutional formulae for the acyclic saturated hydrocarbons substituted by the same halogen atoms Cl or Br ("polyhaloalkanes"), in which hydrogen atoms are omitted. In this paper, all "polyhaloalkanes" include alkanes and monohaloalkanes, all "polyhaloalkyls" include alkyls and monohaloakyls. We call generally them "polyhaloalkanes" and "polyhaloalkyls".

Each point of degree 1—4 represents a carbon atom. Each point of degree 1 represents a chlorine atom (or bromine atom), hydrogen atoms being omitted. Each line jioning two points represents a single covalent bond.

Table 1. The numbers of constitutions of "polyhaloalkyls" $C_iH_{2i+1-j}X_j$ (a_{ij})

j \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14
0	1	1	2	4	8	17	39	89	211	507	1238	3057	7639	19241
1	1	2	5	12	31	80	210	555	1479	3959	10652	28760	77910	211624
2	1	3	9	27	81	240	711	2094	6152	18012	52613	153297	445772	1293780
3	1	3	12	44	154	525	1753	5741	18548	59211	187167	586653	1825527	5644631
4		2	12	55	232	912	3436	12515	44429	154424	527570	1776175	5905873	19426252
5		1	9	55	282	1295	5549	22568	88256	334489	1235865	4470252	15881266	55554722
6			5	44	282	1539	7569	34564	149460	619157	2478146	9640588	36618844	136281985
7			2	27	232	1539	8811	45594	219268	996800	4333832	18168198	73886219	292835749
8				12	154	1295	8811	52266	281676	1412485	6695383	30327368	132310490	559271564
9				4	81	912	7569	52266	318785	1775118	9217067	45265437	212398483	959395756
10					31	525	5549	45594	318785	1987802	11372557	60812370	307880633	1489712231
11					8	240	3436	34564	281676	1987802	12621710	73869420	405073721	2105736302
12						80	1753	22568	219268	1775118	12621710	81359477	485467506	2720805802
13						17	711	12515	149460	1412485	11372557	81359477	531174067	3222812516
14							210	5741	88256	996800	9217067	73869420	531174067	3505992799
15							39	2094	44429	619157	6695383	60812370	485467506	3505992799
16								555	18548	334489	4333832	45265437	405073721	3222812516
17								89	6152	154424	2478146	30327368	307880633	2720805802
18									1479	59211	1235865	18168198	212398483	2105736302
19									211	18012	527570	9640588	132310490	1489712231
20										3959	187167	4470252	73886219	959395756
21										507	52613	1776175	36618844	559271564
22											10652	586653	15881266	292835749
23											1238	153297	5905873	136281985
24												28760	1825527	55554722
25												3057	445772	19426252
26													77910	5644631
27													7639	1293780
28														211624
29														19241

When $j=0$, a_{i0} is the number of constitutions of alkyls

1.2 Planted quartic tree with two different kinds of points

A planted quartic tree with two different kinds of points is a quartic tree with two different kinds of points that besides the above–mentioned two kinds of points has a distinguishable point, which has degree 1–3, this point is called a root. There is a direct correspodence between planted quartic trees with two different kinds of points and constitutional formalae of "polyhaloalkyls".

1.3 Steric tree with two different kinds of points

A steric tree with two different kinds of points is a quartic tree, in which four neighbors (neighbouring points) of every carbon point are given a tetrahedral configuration.

A steric tree with two different kinds of points represents a configurational formula of a "polyhaloalkane".

1.4 Similarly, a planted steric tree with two different kinds of points is a steric tree which also contains a

Table 2. The numbers of constitutions of "polyhaloalkanes" $C_iH_{2i+2-j}X_j$ (b_{ij})

j \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14
0	1	1	1	2	3	5	9	18	35	75	159	355	802	1858
1	1	1	2	4	8	17	39	89	211	507	1238	3057	7639	19241
2	1	2	4	9	21	52	129	332	859	2261	5983	15976	42836	115469
3	1	2	5	14	39	109	312	890	2552	7325	21047	60465	173750	499068
4	1	2	6	20	62	198	625	1972	6169	19226	59513	183397	562266	1716593
5		1	5	20	78	287	1031	3612	12432	42098	140718	464912	1520832	4931131
6		1	4	20	87	367	1475	5736	21618	79599	286925	1016459	3546076	12208953
7			2	14	78	390	1806	7861	32743	131492	512730	1950338	7264842	26575036
8			1	9	62	367	1940	9515	43840	192651	814002	3330739	13262417	51597661
9				4	39	287	1806	10100	52039	251607	1156993	5106503	21782822	90270074
10				2	21	198	1475	9515	55131	295006	1482035	7078709	32425551	143409568
11					8	109	1031	7861	52039	310790	1716540	8909969	43970225	208045876
12					3	52	625	5736	43840	295006	1802538	10218213	54523902	276784514
13						17	312	3612	32743	251607	1716540	10692600	61974936	338698841
14						5	129	1972	21618	192651	1482035	10218213	64669834	382017997
15							39	890	12432	131492	1156993	8909969	61974936	397598614
16							9	332	6169	79599	814002	7078709	54523902	382017997
17								89	2552	42098	512730	5106503	43970225	338698841
18								18	859	19226	286925	3330739	32425551	276784514
19									211	7325	140718	1950338	21782822	208045876
20									35	2261	59513	1016459	13262417	143409568
21										507	21047	464912	7264842	90270074
22										75	5983	183397	3546076	51597661
23											1238	60465	1520832	26575036
24											159	15976	562266	12208953
25												3057	173750	4931131
26												355	42836	1716593
27													7639	499068
28													802	115469
29														19241
30														1858

When $j=0$, b_{i0} is the number of constitutions of alkanes

distinguishable root point besides the above-mentioned two kinds of points. There is a direct correspondence between the planted steric trees with two different kinds of points and configurations of "polyhaloalkyls".

2. COUNTING

2.1 Let $A(x,y)$ be the generating function of counting the planted trees with two different kinds of points, in which the coefficient a_{ij} of the term x^iy^j is the number of constitutions of "polyhaloalkyls" containing i carbon atoms and j halogen atoms. We establish the recurrence formula

$$A(x,y)=\sum_{i=0}^{\infty}\sum_{j=0}^{2i+1}a_{ij}x^iy^j$$

$$=1+y+\frac{1}{6}x[A^3(x,y)+3A(x,y)A(x^2,y^2)+2A(x^3,y^3)], \qquad (1)$$

Table 3. The numbers of configurations of "polyhaloalkyls" $C_iH_{2i+1-j}X_j$ (c_{ij})

j \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14
0	1	1	2	5	11	28	74	199	551	1553	4436	12832	37496	110500
1	1	3	8	23	69	208	636	1963	6099	19059	59836	188576	596252	1890548
2	1	4	16	60	219	786	2784	9766	34005	117704	405456	1391102	4756734	16218370
3	1	4	22	106	471	2000	8186	32588	126999	486496	1837584	6860140	25358224	92944164
4		3	22	138	758	3814	18056	81636	356126	1509807	6253118	25399588	101488764	399848734
5		1	16	138	952	5742	31608	162750	796166	3739777	16995732	75149706	324691474	1375391286
6			8	106	952	7006	45284	267066	1470322	7670088	38309812	184605518	863166494	3933589322
7			2	60	758	7006	53996	368052	2293302	13335768	73394770	386141572	1956538368	9601974442
8				23	471	5742	53996	430924	3063438	19963754	121512430	699826462	3850031686	20377327548
9				5	219	3814	45284	430924	3533824	25993522	175836540	1112474634	6662192350	38102764386
10					69	2000	31608	368052	3533824	29617416	224091632	1564505790	10232752500	63396954834
11					11	786	18056	267066	3063438	29617416	252696670	1957906438	14043947930	94546293092
12						208	8186	162750	2293302	25993522	252696670	2188358762	17302541536	127053438404
13						28	2784	81636	1470322	19963754	224091632	2188358762	19191788200	154419537474
14							636	32588	796166	13335768	175836540	1957906438	19191788200	170142334656
15							74	9766	356126	7670088	121512430	1564505790	17302541536	170142334656
16								1963	126999	3739777	73394770	1112474634	14043947930	154419537474
17								199	34005	1509807	38309812	699826462	10232752500	127053438404
18									6099	486496	16995732	386141572	6662192350	94546293092
19									551	117704	6253118	184605518	3850031686	63396954834
20										19059	1837584	75149706	1956538368	38102764386
21										1553	405456	25399588	863166494	20377327548
22											59836	6860140	324691474	9601974442
23											4436	1391102	101488764	3933589322
24												188576	25358224	1375391286
25												12832	4756734	399848734
26													596252	92944164
27													37496	16218370
28														1890548
29														110500

When $j=0$, c_{i0} is the number of configurations of alkyls

where $a_{00}=1$ and $a_{01}=1$.

The numerical results are given in Table 1 (all numbers for $i=0$ are omitted in each table).

2.2 Let $B(x,y)$ be the generating function of counting the quartic trees with two different kinds of points, in which the coefficient b_{ij} of the term x^iy^j is the number of constitutions of "polyhaloalkanes" containing i carbon atoms and j halogen atoms. Using the method of Harary et al. (see Refs. 3,4.), we can obtain the function

$$B(x,y)=\sum_{i=0}^{\infty}\sum_{j=0}^{2i+2}b_{ij}x^iy^j$$

$$=\frac{1}{24}x[A^4(x,y)+6A^2(x,y)A(x^2,y^2)+3A^2(x^2,y^2)+8A(x,y)A(x^3,y^3)$$

$$+6A(x^4,y^4)]-\frac{1}{2}[A_1^2(x,y)-A_1(x^2,y^2)], \qquad (2)$$

Table 4. The numbers of configurations of "polyhaloalkanes" $C_iH_{2i+2-j}X_j$ (d_{ij})

j \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14
0	1	1	1	2	3	5	11	24	55	136	345	900	2412	6563
1	1	1	2	5	11	28	74	199	551	1553	4436	12832	37496	110500
2	1	2	5	13	37	108	325	993	3070	9564	29979	94392	298311	945592
3	1	2	6	22	77	270	950	3310	11477	39630	136252	466818	1594582	5432346
4	1	2	8	33	134	544	2172	8508	32829	124903	469494	1746443	6438002	23546146
5		1	6	34	176	852	3932	17466	75224	315897	1298894	5246282	20868790	81923064
6		1	5	33	200	1127	5971	29949	143843	666588	2998195	13149996	56448917	237860683
7			2	22	176	1220	7572	43366	233636	1198732	5909906	28184110	130675662	591397876
8			1	13	134	1127	8226	54044	327874	1868264	10119689	52565293	263581046	1282452558
9				5	77	852	7572	58022	400168	2547462	15219890	86347296	469196868	2457930054
10				2	37	544	5971	54044	427690	3061609	20270742	126038623	744070341	4204946588
11					11	270	3932	43366	400168	3253100	24024926	164466000	1058369938	6468502302
12					3	108	2172	29949	327874	3061609	25418776	192648001	1356908880	8996479486
13						28	950	17466	233636	2547462	24024926	203021036	1573088992	11357085350
14						5	325	8508	143843	1868264	20270742	192648001	1652225542	13047940632
15							74	3310	75224	1198732	15219890	164466000	1573088992	13663432888
16							11	993	32829	666588	10119689	126038623	1356908880	13047940632
17								199	11477	315897	5909906	86347296	1058369938	11357085350
18								24	3070	124903	2998195	52565293	744070341	8996479486
19									551	39630	1298894	28184110	469196868	6468502302
20									55	9564	469494	13149996	263581046	4204946588
21										1553	136252	5246282	130675662	2457930054
22										136	29979	1746443	56448917	1282452558
23											4436	466818	20868790	591397876
24											345	94392	6438002	237860683
25												12832	1594582	81923064
26												900	298311	23546146
27													37496	5432346
28													2412	945592
29														110500
30														6563

When $j=0$, d_{i0} is the number of configurations of alkanes

where $A_1(x,y) = A(x,y) - y - 1.$ (3)

The numerical results are given in Table 2.

2.3 Let C(x,y) be the generating function of counting the planted steric trees with two different kinds of points, in which the coefficient c_{ij} of the term x^iy^j is the number of configuration of "polyhaloalkyls" containing i carbon atoms and j halogen atoms. We establish the recurrence formula

$$C(x,y) = \sum_{i=0}^{\infty}\sum_{j=0}^{2i+1} c_{ij}x^iy^j$$

$$= 1 + y + \frac{1}{3}x[C^3(x,y) + 2C(x^3,y^3)], \quad (4)$$

where $c_{00} = 1$ and $c_{01} = 1.$

The c_{ij} is the number of configurations of "polyhaloalkyls" containing i carbon atoms and j halogen

Table 5. The numbers of achiral configurations of "polyhaloalkyls" $C_iH_{2i+1-j}X_j$ (e_{ij})

j \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14
0	1	1	2	3	5	8	14	23	41	69	122	208	370	636
1	1	1	2	3	5	8	14	23	41	69	122	208	370	636
2	1	2	4	8	17	32	64	120	235	438	848	1572	3012	5568
3	1	2	4	8	17	32	64	120	235	438	848	1572	3012	5568
4		1	4	10	26	60	140	300	660	1365	2896	5856	12124	24120
5		1	4	10	26	60	140	300	660	1365	2896	5856	12124	24120
6			2	8	26	72	198	488	1210	2788	6506	14364	32198	69016
7			2	8	26	72	198	488	1210	2788	6506	14364	32198	69016
8				3	17	60	198	570	1610	4158	10732	25960	63186	146208
9				3	17	60	198	570	1610	4158	10732	25960	63186	146208
10					5	32	140	488	1610	4732	13648	36432	96824	242784
11					5	32	140	488	1610	4732	13648	36432	96824	242784
12						8	64	300	1210	4158	13648	40688	119134	325804
13						8	64	300	1210	4158	13648	40688	119134	325804
14							14	120	660	2788	10732	36432	119134	358800
15							14	120	660	2788	10732	36432	119134	358800
16								23	235	1365	6506	25960	96824	325804
17								23	235	1365	6506	25960	96824	325804
18									41	438	2896	14364	63186	242784
19									41	438	2896	14364	63186	242784
20										69	848	5856	32198	146208
21										69	848	5856	32198	146208
22											122	1572	12124	69016
23											122	1572	12124	69016
24												208	3012	24120
25												208	3012	24120
26													370	5568
27													370	5568
28														636
29														636

When $j=0$, e_{i0} is the number of achiral configurations of alkyls

atoms. The results are given in Table 3.

2.4 Let D(x,y) be the generating function of counting steric trees with two different kinds of points. Using the method of Harary et al. (see Refs. 3,4.), we can obtain the following function:

$$D(x,y)=\sum_{i=0}^{\infty}\sum_{j=0}^{2i+2} d_{ij}x^i y^j$$

$$=\frac{1}{12}x[C^4(x,y)+3C^2(x^2,y^2)+8C(x,y)C(x^3,y^3)]$$

$$-\frac{1}{2}[C_1^2(x,y)-C_1(x^2,y^2)], \tag{5}$$

where $C_1(x,y)=C(x,y)-y-1.$ (6)

The d_{ij} is the numbers of configurations of "polyhalolkanes" containing i carbon atoms and j halogen atoms. The results are given in Table 4.

Table 6. The numbers of chiral configurations of "polyhaloalkyls" $C_iH_{2i+1-j}X_j$ (f_{ij})

j \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14
0	0	0	0	2	6	20	60	176	510	1484	4314	12624	37126	109864
1	0	2	6	20	64	200	622	1940	6058	18990	59714	188368	595882	1889912
2	0	2	12	52	202	754	2720	9646	33770	117266	404608	1389530	4753722	16212802
3	0	2	18	98	454	1968	8122	32468	126764	486058	1836736	6858568	25355212	92938596
4		2	18	128	732	3754	17916	81336	355466	1508442	6250222	25393732	101476640	399824614
5		0	12	128	926	5682	31468	162450	795506	3738412	16992836	75143850	324679350	1375367166
6			6	98	926	6934	45086	266578	1469112	7667300	38303306	184591154	863134296	3933520306
7			0	52	732	6934	53798	367564	2292092	13332980	73388264	386127208	1956506170	9601905426
8				20	454	5682	53798	430354	3061828	19959596	121501698	699800502	3849968500	20377181340
9				2	202	3754	45086	430354	3532214	25989364	175825808	1112448674	6662129164	38102618178
10					64	1968	31468	367564	3532214	29612684	224077984	1564469358	10232655676	63396712050
11					6	754	17916	266578	3061828	29612684	252683022	1957870006	14043851106	94546050308
12						200	8122	162450	2292092	25989364	252683022	2188318074	17302422402	127053112600
13						20	2720	81336	1469112	19959596	224077984	2188318074	19191669066	154419211670
14							622	32468	795506	13332980	175825808	1957870006	19191669066	170141975856
15							60	9646	355466	7667300	121501698	1564469358	17302422402	170141975856
16								1940	126764	3738412	73388264	1112448674	14043851106	154419211670
17								176	33770	1508442	38303306	699800502	10232655676	127053112600
18									6058	486058	16992836	386127208	6662129164	94546050308
19									510	117266	6250222	184591154	3849968500	63396712050
20										18990	1836736	75143850	1956506170	38102618178
21										1484	404608	25393732	863134296	20377181340
22											59714	6858568	324679350	9601905426
23											4314	1389530	101476640	3933520306
24												188368	25355212	1375367166
25												12624	4753722	399824614
26													595882	92938596
27													37126	16212802
28														1889912
29														109864

When $j=0$, f_{i0} is the number of chiral configurations of alkyls

2.5 Let E(x,y) be the generating function of counting achiral planted steric trees with two different kinds of points. Let F(x,y) be the generating function of counting chiral planted steric trees with two different kinds of points. We get the functional relations

$$E(x,y)+\frac{1}{2}F(x,y)=1+y+\frac{1}{6}x[C^3(x,y)+3E(x,y)C(x^2,y^2)+2C(x^3,y^3)] \tag{7}$$

and

$$E(x,y)+F(x,y)=C(x,y). \tag{8}$$

From (7),(8) and (4) we get

$$E(x,y)=\sum_{i=0}^{\infty}\sum_{j=0}^{2i+1}e_{ij}x^iy^j$$

$$=1+y+xE(x,y)\,C(x^2,y^2), \tag{9}$$

Table 7. The numbers of achiral configurations of "polyhaloalkanes" $C_iH_{2i+2-j}X_j$ (g_{ij})

j \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14
0	1	1	1	2	3	5	7	14	21	40	61	118	186	355
1	1	1	2	3	5	8	14	23	41	69	122	208	370	636
2	1	2	3	7	11	24	39	83	138	288	485	994	1691	3420
3	1	2	4	8	17	32	64	120	235	438	848	1572	3012	5568
4	1	2	4	11	22	54	102	240	449	1011	1872	4107	7572	16236
5		1	4	10	26	60	140	300	660	1365	2896	5856	12124	24120
6		1	3	11	26	77	169	447	935	2312	4701	11110	22161	50661
7			2	8	26	72	198	488	1210	2788	6506	14364	32198	69016
8			1	7	22	77	198	598	1412	3852	8619	22069	47700	116640
9				3	17	60	198	570	1610	4158	10732	25960	63186	146208
10				2	11	54	169	598	1610	4921	12190	34067	80005	210300
11					5	32	140	488	1610	4732	13648	36432	96824	242784
12					3	24	102	447	1412	4921	13648	42063	107990	306936
13						8	64	300	1210	4158	13648	40688	119134	325804
14						5	39	240	935	3852	12190	42063	119134	369300
15							14	120	660	2788	10732	36432	119134	358800
16							7	83	449	2312	8619	34067	107990	369300
17								23	235	1365	6506	25960	96824	325804
18								14	138	1011	4701	22069	80005	306936
19									41	438	2896	14364	63186	242784
20									21	288	1872	11110	47700	210300
21										69	848	5856	32198	146208
22										40	485	4107	22161	116640
23											122	1572	12124	69016
24											61	994	7572	50661
25												208	3012	24120
26												118	1691	16236
27													370	5568
28													186	3420
29														636
30														355

When j=0, g_{i0} is the number of achiral configurations of alkanes

where $e_{00} = 1$ and $e_{01} = 1$.

The e_{ij} is the number of achiral configurations of "polyhaloalkyls" containing i carbon atoms and j halogen atoms. The results are given in Table 5.

From (8) we get

$$F(x,y) = \sum_{i=0}^{\infty} \sum_{j=0}^{2i+1} f_{ij} x^i y^j$$
$$= D(x,y) - E(x,y), \tag{10}$$

where f_{ij} is the number of chiral configurations of "polyhaloalkyls" containing i carbon atoms and j halogen atoms. The results are given in Table 6.

2.6. Let G(x,y) be the generating function of counting achiral steric trees with two different kinds of

Table 8. The numbers of chiral configurations of polyhaloalkanes[a] $C_iH_{2i+2-j}X_j$ (h_{ij})

j \ i	1	2	3	4	5	6	7	8	9	10	11	12	13	14
0	0	0	0	0	0	0	4	10	34	96	284	782	2226	6208
1	0	0	0	2	6	20	60	176	510	1484	4314	12624	37126	109864
2	0	0	2	6	26	84	286	910	2932	9276	29494	93398	296620	942172
3	0	0	2	14	60	238	886	3190	11242	39192	135404	465246	1591570	5426778
4	0	0	4	22	112	490	2070	8268	32380	123892	467622	1742336	6430430	23529910
5		0	2	24	150	792	3792	17166	74564	314532	1295998	5240426	20856666	81898944
6		0	2	22	174	1050	5802	29502	142908	664276	2993494	13138886	56426756	237810022
7			0	14	150	1148	7374	42878	232426	1195944	5903400	28169746	130643464	591328860
8			0	6	112	1050	8028	53446	326462	1864412	10111070	52543224	263533346	1282335918
9				2	60	792	7374	57452	398558	2543304	15209158	86321336	469133682	2457783846
10				0	26	490	5802	53446	426080	3056688	20258552	126004556	743990336	4204736288
11					6	238	3792	42878	398558	3248368	24011278	164429568	1058273114	6468259518
12					0	84	2070	29502	326462	3056688	25405128	192605938	1356800890	8996172550
13						20	886	17166	232426	2543304	24011278	202980348	1572969858	11356759546
14						0	286	8268	142908	1864412	20258552	192605938	1652106408	13047571332
15							60	3190	74564	1195944	15209158	164429568	1572969858	13663074088
16							4	910	32380	664276	10111070	126004556	1356800890	13047571332
17								176	11242	314532	5903400	86321336	1058273114	11356759546
18								10	2932	123892	2993494	52543224	743990336	8996172550
19									510	39192	1295998	28169746	469133682	6468259518
20									34	9276	467622	13138886	263533346	4204736288
21										1484	135404	5240426	130643464	2457783846
22										96	29494	1742336	56426756	1282335918
23											4314	465246	20856666	591328860
24											284	93398	6430430	237810022
25												12624	1591570	81898944
26												782	296620	23529910
27													37126	5426778
28													2226	942172
29														109864
30														6208

When j = 0, h_{i0} is the number of chiral configurations of alkanes

points. Let H(x,y) be the generating function of counting chiral steric trees with two different kinds of points. Then,

$$G(x,y) + H(x,y) = D(x,y). \tag{11}$$

Using the method of Harary et al., we can obtain the following functional relations:

$$R(x,y) = \frac{1}{24}x[C^4(x,y) + 6E^2(x,y)C(x^2,y^2) + 3C^2(x^2,y^2) + 8C(x,y)C(x^3,y^3) + 6C(x^4,y^4)], \tag{12}$$

$$D'(x,y) = \frac{1}{12}x[C^4(x,y) + 3C^2(x^2,y^2) + 8C(x,y)C(x^3,y^3)], \tag{13}$$

$$P(x,y) = 2R(x,y) - D'(x,y)$$

$$= \frac{1}{2} x[E^2(x,y)C(x^2,y^2) + C(x^4,y^4)], \tag{14}$$

$$Q(x,y) = \frac{1}{2}[E_1^2(x,y) + E_1(x^2,y^2)], \tag{15}$$

$$E_1(x,y) = E(x,y) - y - 1, \tag{16}$$

$$S(x,y) = \frac{1}{2}[C_1(x^2,y^2) + E_1(x^2,y^2)] \tag{17}$$

and

$$\begin{aligned} G(x,y) &= \sum_{i=0}^{\infty} \sum_{j=0}^{2i+2} g_{ij} x^i y^j \\ &= P(x,y) - Q(x,y) + S(x,y) \\ &= \frac{1}{2}[xC(x^4,y^4) + C_1(x^2,y^2) + yE(x,y) + E(x,y) - (y+1)^2], \end{aligned} \tag{18}$$

where g_{ij} is the number of achiral configurations of "polyhaloalkanes" containing i carbon atoms and j halogen atoms. The results are given in Table 7.

From (11) we get

$$\begin{aligned} H(x,y) &= \sum_{i=0}^{\infty} \sum_{j=0}^{2i+2} h_{ij} x^i y^j \\ &= D(x,y) - G(x,y), \end{aligned} \tag{19}$$

where h_{ij} is the number of chiral configurations of "polyhaloalkanes" containing i carbon atoms and j halogen atoms. The results are given in Table 8.

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