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The Numbers of Structural Isomers, Stereoisomers, and Chiral and Achiral Stereoisomers of Fluorochloroalkanes

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Three recurrence formulas are presented for counting structural isomers, stereoisomers, and achiral stereoisomers of "fluorochloroalkyls", $C_iH_{2i+1-j-k}Cl_jF_k$ (j = 0–2i + 1; k = 0–2i + 1 – j). A generating function for counting chiral stereoisomers of fluorochloroalkyls, $C_iH_{2i+1-j-k}Cl_jF_k$, and four generating functions for counting structural isomers, stereoisomers, and achiral and chiral stereoisomers of fluorochloroalkanes, $C_iH_{2i+2-j-k}Cl_jF_k$ (j = 0–2i + 2; k = 0–2i + 2 – j) are obtained. Some results are tabulated.

The enumerations of structural isomers, stereoisomers, chiral stereoisomers, and achiral stereoisomers of some acyclic compounds have been reported.[1–7] In particular, Read[4] has discussed fully and clearly the enumerations of structural isomers and stereoisomers of acyclic compounds. However, the enumeration of isomers of fluorochloroalkanes has not been reported yet, though they are useful in many aspects.

We present three recurrence formulas for counting structural isomers, stereoisomers, and achiral stereoisomers of fluorochloroalkyls and obtain the numbers of structural isomers, stereoisomers, and chiral and achiral stereoisomers of fluorochloroalkanes using Pólya's theorem.[4,6]

1. DEFINITIONS

1.1. Quartic Tree with Three Different Kinds of Points. Consider a tree T which consists of a finite set of three different kinds of points. One kind of point has a degree of 1–4 and is colored black, representing the carbon atom; the second kind of point has only degree 1 and is colored red, representing fluorine atoms; and the third kind of point also has only degree 1 and is colored blue, representing chlorine atoms. The number of points cán be an arbitrary natural number. The tree is called a quartic tree with three different kinds of points. Quartic trees with three different kinds of points represent structural formulas for the acyclic saturated hydrocarbons substituted by two kinds of halogen atoms Cl and F (fluorochloroalkanes), in which hydrogen atoms are omitted. In this paper, all fluorochloroalkanes include alkanes (j = 0 and k = 0), fluoroalkanes, chloroalkanes, and fluorochloroalkanes; all fluorochloroalkyls include alkyls, fluoroalkyls, chloroalkyls, and fluorochloroalkyls.

1.2. Planted Quartic Tree with Three Different Kinds of Points. A planted quartic tree with three different kinds of points is a quartic tree with three different kinds of points, in which, beside those points, there is a distinguishable point, with a degree 1–3; this point is called a root. There is a direct correspondence between planted quartic trees with three different kinds of points and structural formulas of fluorochloroalkyls.

1.3. Steric Tree with Three Different Kinds of Points. A steric tree with three different kinds of points is a quartic tree in which every carbon point has four neighbors (neighboring points) in a tetrahedral configuration.

A steric tree with three different kinds of points represents a stereostructural formula of a fluorochloroalkane.

1.4. A planted steric tree with three different kinds of points is a steric tree which contains a distinguishable root point. There is a direct correspondence between the planted steric trees with three different kinds of points and stereoisomers of fluorochloroalkyls.

2. COUNTING

2.1. Let $A(x,y,z)$ be the generating function for counting the planted trees with three different kinds of points, in which the coefficient $a(i,j,k)$ of the term $x^iy^jz^k$ is the number of structural isomers of fluorochloroalkyls containing i carbon atoms, j chlorine atoms, and k fluorine atoms. We establish the recurrence formula

$$A(x,y,z) = \sum_{i=0}^{\infty}\sum_{j=0}^{2i+1}\sum_{k=0}^{2i+1-j} a(i,j,k)x^iy^jz^k = 1 + y + z + {}^1/_6x[A^3(x,y,z) + 3A(x,y,z)A(x^2,y^2,z^2) + 2A(x^3,y^3,z^3)] \quad (1)$$

where $a(0,0,0) = 1$, $a(0,0,1) = 1$, $a(0,1,0) = 1$, and $a(i,j,k) = a(i,k,j) = a(i,j,2i+1-j-k) = a(i,k,2i+1-j-k) = a(i,2i+1-j-k,j) = a(i,2i+1-j-k,k)$.

2.2. Let $B(x,y,z)$ be the generating function for counting the quartic trees with three different kinds of points, in which the coefficient $b(i,j,k)$ of the term $x^iy^jz^k$ is the number of structural isomers of fluorochloroalkanes containing i carbon atoms, j chlorine atoms and k fluorine atoms. Using the method of Harary et al.,[3,4] we can obtain the function

$$B(x,y,z) = \sum_{i=1}^{\infty}\sum_{j=0}^{2i+2}\sum_{k=0}^{2i+2-j} b(i,j,k)x^iy^jz^k = {}^1/_{24}x[A^4(x,y,z) + 6A^2(x,y,z)A(x^2,y^2,z^2) + 3A^2(x^2,y^2,z^2) + 8A(x,y,z)A(x^3,y^3,z^3) + 6A(x^4,y^4,z^4)] - {}^1/_2[A^2{}_1(x,y,z) - A_1(x^2,y^2,z^2)] \quad (2)$$

where

$$A_1(x,y,z) = A(x,y,z) - y - z - 1 \quad (3)$$

and $b(i,j,k) = b(i,k,j) = b(i,j,2i+2-j-k) = b(i,k,2i+2-j-k) = b(i,2i+2-j-k,j) = b(i,2i+2-j-k,k)$.

2.3. Let $C(x,y,z)$ be the generating function for counting the planted steric trees with three different kinds of points, in which the coefficient $c(i,j,k)$ of the term $x^iy^jz^k$ is the number of stereoisomers of fluorochloroalkyls containing i carbon

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atoms, j chlorine atoms, and k fluorine atoms. We establish the recurrence formula

$$C(x,y,z) = \sum_{i=0}^{\infty} \sum_{j=0}^{2i+1} \sum_{j=0}^{2i+1-j} c(i,j,k)x^i y^j z^k = 1 + y + z + {}^1/_3 x[C^3(x,y,z) + 2C(x^3,y^3,z^3)] \quad (4)$$

where $c(0,0,0) = 1$, $c(0,0,1) = 1$, $c(0,1,0) = 1$, and $c(i,j,k) = c(i,k,j) = c(i,j,2i + 1 - j - k) = c(i,k,2i + 1 - j - k) = c(i,2i + 1 - j - k,j) = c(i,2i + 1 - j - k,k)$.

The $c(i,j,k)$ is the number of stereoisomers of fluorochloroalkyls containing i carbon atoms, j chlorine atoms, and k fluorine atoms.

2.4. Let $D(x,y,z)$ be the generating function for counting steric trees with three different kinds of points. Using the method of Harary et al.,[3,4] we can obtain the following function:

$$D(x,y,z) = \sum_{i=1}^{\infty} \sum_{j=0}^{2i+2} \sum_{j=0}^{2i+2-j} d(i,j,k)x^i y^j z^k = {}^1/_{12} x[C^4(x,y,z) + 3C^2(x^2,y^2,z^2) + 8C(x,y,z)C(x^3,y^3,z^3)] - {}^1/_2[C_1^2(x,y,z) - C_1(x^2,y^2,z^2)] \quad (5)$$

where

$$C_1(x,y,z) = C(x,y,z) - y - z - 1 \quad (6)$$

Here, $d(i,j,k)$ is the number of stereoisomers of fluorochloroalkanes containing i carbon atoms, j chlorine atoms, and k fluorine atoms, and $d(i,j,k) = d(i,k,j) = d(i,j,2i + 2 - j - k) = d(i,k,2i + 2 - j - k) = d(i,2i + 2 - j - k,j) = d(i,2i + 2 - j - k,k)$.

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

$$E(x,y,z) + {}^1/_2 F(x,y,z) = 1 + y + z + {}^1/_6 x[C^3(x,y,z) + 3E(x,y,z)C(x^2,y^2,z^2) + 2C(x^3,y^3,z^3)] \quad (7)$$

and

$$E(x,y,z) + F(x,y,z) = C(x,y,z) \quad (8)$$

From eqs 4, 7, and 8 we get

$$E(x,y,z) = \sum_{i=0}^{\infty} \sum_{j=0}^{2i+1} \sum_{j=0}^{2i+1-j} e(i,j,k)x^i y^j z^k = 1 + y + z + xE(x,y,z)C(x^2,y^2,z^2) \quad (9)$$

where $e(0,0,0) = 1$, $e(0,0,1) = 1$, $e(0,1,0) = 1$, and $e(i,j,k) = e(i,k,j) = e(i,j,2i + 1 - j - k) = e(i,k,2i + 1 - j - k) = e(i,2i + 1 - j - k,j) = e(i,2i + 1 - j - k,k)$.

Here, $e(i,j,k)$ is the number of achiral stereoisomers of fluorochloroalkyls containing i carbon atoms, j chlorine atoms, and k fluorine atoms. The results are given in Table I.

From eq 8 we get

$$F(x,y,z) = \sum_{i=0}^{\infty} \sum_{j=0}^{2i+1} \sum_{j=0}^{2i+1-j} f(i,j,k)x^i y^j z^k = C(x,y,z) - E(x,y,z) \quad (10)$$

where $f(i,j,k)$ is the number of chiral stereoisomers of fluorochloroalkyls containing i carbon atoms, j chlorine atoms, and k fluorine atoms, and $f(i,j,k) = f(i,k,j) = f(i,j,2i + 1 - j - k) = f(i,k,2i + 1 - j - k) = f(i,2i + 1 - j - k,j) = f(i,2i + 1 - j - k,k)$.

2.6. Let $G(x,y,z)$ be the generating function of achiral stereoisomer of fluorochloroalkanes and $D'(x,y,z)$ be the generating function of stereoisomer of fluorochloroalkanes containing one labeled carbon atom. Let $P(x,y,z)$ be the generating function of achiral stereoisomer of fluorochloroalkanes containing one labeled carbon atom and let $D_2(x,y,z)$ be the generating function of chiral stereoisomer of fluorochloroalkanes containing one labeled carbon atom. Then

$$D'(x,y,z) = P(x,y,z) + D_2(x,y,z) \quad (11)$$

Let

$$D''(x,y,z) = P(x,y,z) + {}^1/_2 D_2(x,y,z) \quad (12)$$

Then

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

$$D''(x,y,z) = {}^1/_{24} x[C^4(x,y,z) + 3C^2(x^2,y^2,z^2) + 8C(x,y,z)C(x^3,y^3,z^3) + 6E^2(x,y,z)C(x^2,y^2,z^2) + 6C(x^4,y^4,z^4)] \quad (14)$$

and

$$P(x,y,z) = 2D''(x,y,z) - D'(x,y,z) = {}^1/_2 xC(x^4,y^4,z^4) + {}^1/_2 xE^2(x,y,z)C(x^2,y^2,z^2) \quad (15)$$

We must check that $P(x,y,z)$ does not contain meso forms ($R_+ - R_-$).

Let $Q(x,y,z)$ be the generating function of achiral stereoisomer of fluorochloroalkanes containing a labeled C–C bond, in which meso forms are not included. Though meso forms of fluorochloroalkanes containing one labeled C–C bond can be achiral. So

$$Q(x,y,z) = \sum_{i=2}^{\infty} \sum_{j=0}^{2i+2} \sum_{j=0}^{2i+2-j} q(i,j,k)x^i y^j z^k = {}^1/_2[E(x,y,z) - y - z - 1]^2 + {}^1/_2[E(x^2,y^2,z^2) - y^2 - z^2 - 1] \quad (16)$$

Let $S(x,y,z)$ be the generating function of achiral stereoisomer of R–R and R′OR′ forms, in which the meso forms also are not included. So

$$S(x,y,z) = [E(x^2,y^2,z^2) - y^2 - z^2 - 1] \quad (17)$$

However meso forms are achiral and must be counted. Let $M(x,y,z)$ be the generating function of the meso forms of fluorochloroalkanes. Then

$$M(x,y,z) = {}^1/_2[C(x^2,y^2,z^2) - y^2 - z^2 - 1] - {}^1/_2[E(x^2,y^2,z^2) - y^2 - z^2 - 1] \quad (18)$$

and

$$G(x,y,z) = \sum_{i=1}^{\infty} \sum_{j=0}^{2i+2} \sum_{j=0}^{2i+2-j} g(i,j,k)x^i y^j z^k = P(x,y,z) - Q(x,y,z) + S(x,y,z) + M(x,y,z) = {}^1/_2 xC(x^4,y^4,z^4) + {}^1/_2 xE^2(x,y,z)C(x^2,y^2,z^2) - {}^1/_2[E(x,y,z) - y^2 - z^2 - 1]^2 + {}^1/_2[C(x^2,y^2,z^2) - y^2 - z^2 - 1] \quad (19)$$

where $g(i,j,k)$ is the number of achiral stereoisomers of fluorochloroalkanes containing i carbon atoms, j chlorine atoms, and k fluorine atoms. The results are given in Table I.

Table I. Numbers of Isomers of Fluorochloroalkyls and Fluorochloroalkanes[a]

i	j	k	m	$a(i,j,k)$	$c(i,j,k)$	$e(i,j,k)$	$f(i,j,k)$	n	$b(i,j,k)$	$d(i,j,k)$	$g(i,j,k)$	$h(i,j,k)$
1	1	1	1	1	2	0	2	2	1	1	1	0
2	1	1	3	4	8	0	8	4	2	3	1	2
2	1	2	2	5	10	2	8	3	3	4	2	2
2	2	2	1	5	10	2	8	2	4	6	4	2
3	1	1	5	13	32	0	32	6	5	8	2	6
3	1	2	4	23	60	4	56	5	9	16	4	12
3	1	3	3	27	72	0	72	4	12	22	4	18
3	2	2	3	35	100	8	92	4	16	32	8	24
3	2	3	2	35	100	8	92	3	18	36	8	28
4	1	1	7	42	120	0	120	8	12	23	3	20
4	1	2	6	91	300	8	292	7	27	60	8	52
4	1	3	5	138	488	0	488	6	44	106	8	98
4	1	4	4	159	570	10	560	5	55	138	10	128
4	2	2	5	182	700	20	680	6	59	154	22	132
4	2	3	4	251	1020	20	1000	5	86	244	20	224
4	2	4	3	251	1020	20	1000	4	101	290	30	260
4	3	3	3	301	1276	0	1276	4	118	356	20	336
5	1	1	9	131	438	0	438	10	31	69	5	64
5	1	2	8	338	1365	17	1348	9	81	219	17	202
5	1	3	7	620	2788	0	2788	8	154	471	17	454
5	1	4	6	878	4158	26	4132	7	232	758	26	732
5	1	5	5	979	4732	0	4732	6	282	952	26	926
5	2	2	7	829	4060	52	4008	8	207	691	43	648
5	2	3	6	1422	7714	52	7662	7	372	1394	52	1342
5	2	4	5	1840	10430	70	10360	6	527	2092	74	2018
5	2	5	4	1840	10430	70	10360	5	583	2366	70	2296
5	3	3	5	2231	13300	0	13300	6	632	2644	52	2592
5	3	4	4	2586	15806	70	15736	5	814	3570	70	3500
5	4	4	3	2586	15806	70	15736	4	946	4256	106	4150
6	1	1	11	402	1572	0	1572	12	80	208	8	200
6	1	2	10	1200	5856	32	5824	11	240	786	32	754
6	1	3	9	2563	14364	0	14364	10	525	2000	32	1968
6	1	4	8	4263	25960	60	25900	9	912	3814	60	3754
6	1	5	7	5709	36432	0	36432	8	1295	5742	60	5682
6	1	6	6	6287	40688	72	40616	7	1539	7006	72	6934
6	2	2	9	3462	21100	120	20980	10	712	2944	108	2836
6	2	3	8	7047	49170	120	49050	9	1494	7182	120	7062
6	2	4	7	11006	82940	200	82740	8	2482	13010	220	12790
6	2	5	6	13642	106612	200	106412	7	3300	18216	200	18016
6	2	6	5	13642	106612	200	106412	6	3643	20380	272	20108
6	3	3	7	13472	107028	0	107028	8	3012	16708	120	16588
6	3	4	6	19462	165438	200	165238	7	4681	28158	200	27958
6	3	5	5	21910	190432	0	190432	6	5787	36178	200	35978
6	4	4	5	25529	229020	280	228740	6	6748	43498	390	43108
6	4	5	4	25529	229020	280	228740	5	7565	49984	280	49704
7	1	1	13	1218	5568	0	5568	14	210	636	14	622
7	1	2	12	4128	24120	64	24056	13	711	2784	64	2720
7	1	3	11	10020	69016	0	69016	12	1753	8186	64	8122
7	1	4	10	19043	146208	140	146068	11	3436	18056	140	17916
7	1	5	9	29456	242784	0	242784	10	5549	31608	140	31468
7	1	6	8	38002	325804	198	325606	9	7569	45284	198	45086
7	1	7	7	41309	358800	0	358800	8	8811	53996	198	53798
7	2	2	11	13658	101920	280	101640	12	2386	12092	204	11888
7	2	3	10	31999	280584	280	280304	11	5726	34508	280	34228
7	2	4	9	58012	564560	560	564000	10	10841	73174	490	72684
7	2	5	8	84725	878808	560	878248	9	16693	121392	560	120832
7	2	6	7	101932	1089560	688	1088872	8	21516	163001	723	162278
7	2	7	6	101932	1089560	688	1088872	7	23355	179400	688	178712
7	3	3	9	71523	734120	0	734120	10	13299	94884	280	94604
7	3	4	8	122343	1385376	560	1384816	9	23984	190760	560	190200
7	3	5	7	166602	1992976	0	1992976	8	34907	296796	560	296236
7	3	6	6	184350	2243932	688	2243244	7	41935	367900	688	367212
7	4	4	7	195071	2416440	980	2415460	8	40833	359526	1050	358476
7	4	5	6	244298	3157104	980	3156124	7	55399	516536	980	515556
7	4	6	5	244298	3157104	980	3156124	6	61277	581584	1324	580260
7	5	5	5	276507	3663520	0	3663520	6	69217	674152	980	673172
8	1	1	15	3657	19532	0	19532	16	555	1963	23	1940
8	1	2	14	13856	96440	120	96320	15	2094	9766	120	9646
8	1	3	13	37607	315156	0	315156	14	5741	32588	120	32468
8	1	4	12	80087	764904	300	764604	13	12515	81636	300	81336
8	1	5	11	139749	1463280	0	1463280	12	22568	162750	300	162450
8	1	6	10	205120	2282296	488	2281808	11	34564	267066	488	266578
8	1	7	9	256869	2959632	0	2959632	10	45594	368052	488	367564
8	1	8	8	276669	3223994	570	3223424	9	52266	430924	570	430354
8	2	2	13	51640	467040	600	466440	14	7871	48280	480	47800
8	2	3	12	136418	1480962	600	1480362	13	21159	157578	600	156978
8	2	4	11	280153	3452960	1400	3451560	12	44899	382602	1300	381302
8	2	5	10	467550	6283424	1400	6282024	11	78027	731640	1400	730240

Table I. (Continued)

i	j	k	m	$a(i,j,k)$	$c(i,j,k)$	$e(i,j,k)$	$f(i,j,k)$	n	$b(i,j,k)$	$d(i,j,k)$	$g(i,j,k)$	$h(i,j,k)$
8	2	6	9	650517	9226336	2040	9224296	10	114361	1141392	2208	1139184
8	2	7	8	764915	11134160	2040	11132120	9	142969	1479816	2040	1477776
8	2	8	7	764915	11134160	2040	11132120	8	154005	1612282	2610	1609672
8	3	3	11	347462	4513492	0	4513492	12	55458	499196	600	498596
8	3	4	10	682016	10015156	1400	10013756	11	113308	1163152	1400	1161752
8	3	5	9	1078542	17163440	0	17163440	10	188426	2115724	1400	2114324
8	3	6	8	1408556	23457982	2040	23455942	9	261601	3105862	2040	3103822
8	3	7	7	1537621	25989200	0	25989200	8	307276	3747630	2040	3745590
8	4	4	9	1268161	20931624	2940	20928684	10	221301	2577656	3220	2574436
8	4	5	8	1882161	33392884	2940	33389944	9	348577	4412800	2940	4409860
8	4	6	7	2281740	41902660	3680	41898980	8	454452	6028562	4840	6023722
8	4	7	6	2281740	41902660	3680	41898980	7	495633	6677400	3680	6673720
8	5	5	7	2593063	48912080	0	48912080	8	515671	7030940	2940	7028000
8	5	6	6	2879642	55399484	3680	55395804	7	624204	8817320	3680	8813640
8	6	6	5	2879642	55399484	3680	55395804	6	692751	9982942	6158	9976784

[a] i is the number of carbon atoms. j is the number of chlorine atoms. k is the number of fluorine atoms. m is the number of hydrogen atoms of fluorochloroalkyl. n is the number of hydrogen atoms of fluorochloroalkane. $a(i,j,k)$ is the number of structural isomers of fluorochloroalkyls. $c(i,j,k)$ is the number of stereoisomers of fluorochloroalkyls. $e(i,j,k)$ is the number of achiral stereoisomers of fluorochloroalkyls. $f(i,j,k)$ is the number of chiral stereoisomers of fluorochloroalkyls. $b(i,j,k)$ is the number of structural isomers of fluorochloroalkanes. $d(i,j,k)$ is the number of stereoisomers of fluorochloroalkanes. $g(i,j,k)$ is the number of achiral stereoisomers of fluorochloroalkanes. $h(i,j,k)$ is the number of chiral stereoisomers of fluorochloroalkanes.

$-CHClCClF_2$ $\quad$ $-CHFCCl_2F$
$-CClFCHClF$ $\quad$ $-CCl_2CHF_2$
$-CF_2CHCl_2$

Figure 1. Structural isomers of fluorochloroalkyls having a general formula $-C_2HCl_2F_2$; the number is a(2,2,2).

$CH_2ClCClF_2$ $\quad$ $CHCl_2CHF_2$
$CHClFCHClF$ $\quad$ CH_2FCCl_2F

Figure 2. Structural isomers of fluorochloroalkyls having a general formula $C_2H_2Cl_2F_2$; the number is b(2,2,2).

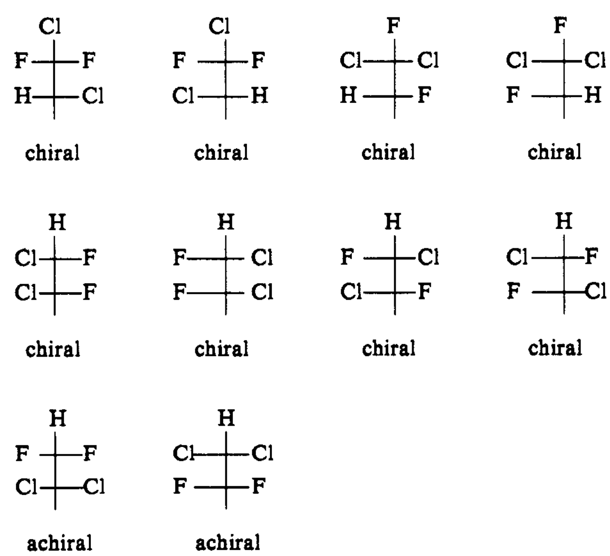

Figure 3. Stereoisomers of fluorochloroalkyls having a general formula $-C_2HCl_2F_2$; the number is c(2,2,2).

Let $H(x,y,z)$ be the generating function of chiral stereoisomers of fluorochloroalkanes, we get

$$H(x,y,z) = \sum_{i=0}^{\infty} \sum_{j=0}^{2i+2} \sum_{j=0}^{2i+2-j} h(i,j,k) x^i y^j z^k = D(x,y,z) - G(x,y,z) \tag{20}$$

where $h(i,j,k)$ is the number of chiral stereoisomers of fluorochloroalkanes containing i carbon atoms, j chlorine atoms, and k fluorine atoms.

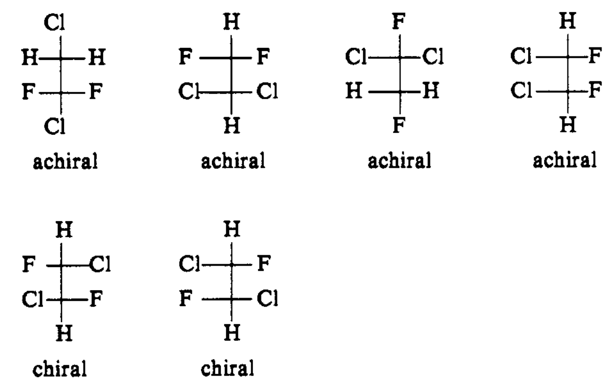

Figure 4. Stereoisomers of fluorochloroalkyls having a general formula $C_2H_2Cl_2F_2$; the number is d(2,2,2).

Some results are given in Table I. As an example, all the structural isomers and stereoisomers (Fischer projections) of the fluorochloroalkyls having the general formula $C_2HCl_2F_2$ and the fluorochloroalkanes having the general formula $C_2H_2Cl_2F_2$ are given in Figures 1–4.

The results for some large molecules may not be perfectly satisfactory from a chemical standpoint because possible steric hindrance is not considered.[8]

REFERENCES AND NOTES

(1) Henze, H. R.; Blair, C. M. The Number of Structurally Isomeric Alcohols of the Methanol Series. *J. Am. Chem. Soc.* **1931**, *53*, 3042.
(2) Henze, H. R.; Blair, C. M. The Number of Structurally Isomeric Hydrocarbons of the Ethylene Series. *J. Am. Chem. Soc.* **1931**, *53*, 3077.
(3) Robinson, R. W.; Harary, F.; Balaban, A. T. The Numbers of Chiral and Achiral Alkanes and Monosubstituted Alkanes. *Tetrahedron* **1976**, *32*, 355.
(4) Read, R. C. In *Chemical Applications of Graph Theory*; Balaban, A. T., Ed.; Academic Press: London, 1976; Chapter 4, p 25.
(5) Wang, J.; Wang, Q. The Numbers of Constitutions, Configurations, Chiral and Achiral Configurations of Polyhaloalkanes $C_iH_{2i+2-j}X_j$. *Tetrahedron* **1991**, *47*, 2969.
(6) Pólya, G.; Kombinatorische Anzahlbestimmungen fur Gruppen, Graphen und Chemische Verbindungen. *Acta Math.* **1937**, *68*, 145.
(7) Wang, J.; Gu, F. Enumeration of Isomers of Polyethers. *J. Chem. Inf. Comput. Sci.* **1991**, *31*, 552.
(8) Klein, D. J. Rigorous Results for Branched Polymer Models with Excluded Volume. *J. Chem. Phys.* **1981**, *75*, 5186.