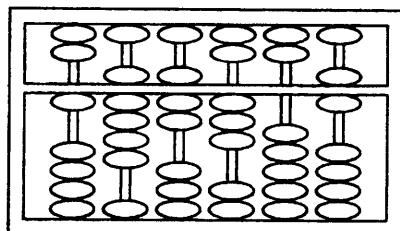


# COMPUTER SCIENCE MONOGRAPHS

*A Publication  
of  
The Institute of Statistical Mathematics*



STATISTICAL DISTRIBUTION OF SYMMETRY GROUPS  
FOR INORGANIC CRYSTAL STRUCTURE DATABASE (ICSD)  
by  
Miyako Fujiwara, Yoshiaki Itoh, Takeo Matsumoto and  
Hiroshi Takeda

# **Computer Science Monographs**

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# Statistical Distribution of Symmetry Groups for Inorganic Crystal Structure Database (ICSD)

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# 1 Introduction

Problems involved in classification of species have been drawing the attention of statisticians. In biological sciences, especially, how to define species is an important problem. Organic compounds can be classified easily by their molecular formulae, but mineral species cannot be classified in a similar manner because of the common presence of solid solution series. Mineral species have been approved by a committee of The International Mineralogical Association by vote. We need a method to define species for general inorganic crystalline substances including minerals on the basis of reasonable criteria without any ambiguity for studying statistical distribution of such species among point groups.

We introduce a method that defines the species (representatives) of inorganic compounds, and studied the statistical distribution of the defined species among space groups (distribution of space groups), by using ICSD (Inorganic Crystal Structure Database (1990)).

ICSD is a database of the CRYSTIN (Crystal Structure Information System), for complete structural information of non-metal inorganic crystals. FIZ Karlsruhe and GMELIN Institute Frankfurt are in charge of making this database, in cooperation with the Institute for Inorganic Chemistry of the University of Bonn.

CRYSTIN includes two other databases. CSD (Cambridge Structural Database, Organic and Organo-Metallic Compounds) made by Cambridge Crystallographic Data Centre, and CRYSTMET (The NRCC Metals Crystallographic Data File, Metallic phases) made by Canadian Scientific Numeric Database Service and National Research Council of Canada.

ICSD includes compound names, chemical formula, unit cell which is a basic element of a compound, atomic position of each atom in the unit cell, symmetry operation parameter which derives entire positions of atoms in the cell from those in an asymmetric unit of the cell, and bibliographic data, etc. Some descriptors in the database are as follows (Table 1.):

ANX	FORMULA TYPE
AUT	AUTHOR'S NAME
CLAS	CRYSTAL CLASS NAME
CODN	CODEN
COL	COLLECTION CODE
CVOL	CELL VOLUME
D	MINIMUM INTERATOMIC DISTANCE
DATE	DATE OF RECORDING OR CORRECTION
ELC	NUMBER OF DIFFERENT CHEMICAL ELEMENTS PRESENT
ELE	KEYWORD
LAST	DESCRIPTOR FOR THE SUBSET SELECTED BY THE LAST 'FIND' COMMAND
LAUE	LAUE CLASS SYMBOL
MINR	MINERAL NAME
PRS	PEARSON SYMBOL
REL	RANGE OF RELATIVE ENTRY NUMBERS
REM	REMARK SYMBOL
RFCD	REFCODE
RVAL	R VALUE RANGE
SGR	SPACE GROUP
SYPR	SYMMETRY PROPERTY
SYST	CRYSTAL SYSTEM

TEST	FLAG
USRN	NAME OF A SAVED SUBSET
YEAR	YEAR OF PUBLICATION

Table 1. List of Descriptors (For more information, See ICSD manual)

The statistical distribution of the symmetry groups has been drawing the attention of crystallographers [1], [8], [9], [10], [11], [12], [13], [14], [15], [16], [17], [18], [19], [20]. Stochastic models are introduced to explain the statistical distribution [5], [7]. Here we make use of the database ICSD and CRYSTMET to study the statistical distribution improving our previous works [2], [3], [4]. Applying the idea of sequential coding [6], we sequentially define species by considering i) space group, ii) chemical component and iii) unit cell volume.

This work was performed on the HITAC M-680 computer (OS/VOS3) at The Institute of Statistical Mathematics. We used ASPEN E2 (Advanced editor System for Programming Environment Extended version 2) as a file editor. In this volume, we call it ASPEN.

## 2 Algorithm

Making use of the ICSD (CRYSTMET) database, we classify crystalline substances by using some of descriptors, define species (representatives) for each class of substances, and obtain the statistical distribution of space groups. Here we use five descriptors of ICSD (CRYSTMET) (Table 2.). We define species sequentially as will be given later.

MINERAL	:	Mineral name
NAME	:	Compound name
FORM	:	Structured chemical formula and empirical formula
CELL	:	Unit cell dimensions, unit cell volume, number of formula units, measured density
SGR	:	Hermann-Mauguin space group symbol

Table 2. Five Descriptors used

We take information on these five descriptors from all the substances in ICSD (CRYSTMET), and copy them into a file. These data are written in small and capital alphanumeric letters of EBCDIC, so that we transform these letters into capital letters of EBCDIK. Then we transform Hermann-Mauguin symbols into 230 Schoenflies symbols and we add the number of lattice point per unit cell to the substance (ITOH4XC. SGRL.FORT(CHARCNV3), Program lists 5.1).

We say two substances are mutually close to each other, when the following three conditions i), ii), and iii) are satisfied.

- i) They have the same space group.
- ii) They have mutually similar chemical formula.

Namely if the ratio for the common elements in both substances,  $WDIF1$ , is more than 75%, these two substances are said to be close to each other.

$$WDIF1 = \frac{ICHEM * 2}{(NC(S_1) + NC(S_2))}$$

where  $NC(S_1)$  is the number of elements included in substance 1,  $NC(S_2)$  is the number of elements in substance 2, and  $ICHEM$  is the number of the common elements of the two substances.

Example.

substance 1 ( $S_1$ ) :  $NaAlSi_3O_8$  , the number of elements = 4 ( $NC(S_1)$ )  
substance 2 ( $S_2$ ) :  $Na_{0.667}K_{0.333}AlSi_3O_8$  , the number of elements = 5 ( $NC(S_2)$ )  
the number of the common elements of the two substances = 4 ( $ICHEM$ )

Hence we obtain

$$WDIF1 = \frac{8}{9} ,$$

in this case.

iii) The primitive unit cell volume of the substances are mutually close to each other.

Consider the following table (Table 3.).

space	lattice	lattice points of unit cell	Primitive lattice volume /unit cell volume
P	Primitive	1	1
C	C-face centered	2	1/2
A	A-face centered	2	1/2
B	B-face centered	2	1/2
I	Body centered	2	1/2
F	All-face centered	4	1/4
R(R)	Rhombohedral setting	1	1
RH	Hexagonal setting(obverse)	3	1/3
RHR	Hexagonal setting(reverse)	3	1/3

Table 3. Lattice Points of Unit Cell

If the following value of  $WDIF2$  for the primitive unit cell volumes of the two substances is smaller than the given value of  $DIFF2$ , we say the two primitive unit cell volumes are mutually close to each other with respect to  $DIFF2$ ,

$$WDIF2 = \frac{|(VOL[S_1] - VOL[S_2])|}{(VOL[S_1] + VOL[S_2])} ,$$

for the primitive unit cell volume of substance 1 ( $S_1$ ),  $VOL[S_1]$ , and for that of substance 2 ( $S_2$ ),  $VOL[S_2]$ .

The procedure of determining the representatives in this method is as follows. Take the necessary information from the ICSD (CRYSTMET) and copy them into a file. When  $N$  substances are already defined to be representatives, we compare the next substance with these  $N$  substances. If this substance is not close to the  $N$  substances, we define this as the  $N + 1$ th representative. If this is close to one of the defined  $N$  substances, we do not define it as the  $N + 1$ th substance. Taking  $DIFF2$  in the above iii), from 0.025 to 0.25 by 0.025, we get the representatives for each case (ITOH4XC.SGRL.FORT(INORDEF4) whose list is given in Program lists 5.2). We print out tables of the distributions of point groups, for the species which we think as representatives of crystalline substances (ITOH4XC. SGRL.FORT(SGRDIST4), Program lists 5.3).

The following Hermann-Mauguin symbols which seems to be unclearly stated in ICSD are not transformed to Schoenflies symbols.

B1N1      BMBM    F13-2/M   I121S  
I12/A1S    IAB       P0       RMH

### **3 User's manual**

The examples of using the following programs are shown in 4.Example.

#### **3.1 Preparation**

Execute ICSD (CRYSTMET) and see the number of the data which satisfy the conditions.

#### **3.2 Input File**

##### **3.2.1 ITOH4XC.@COMMAND.DATA**

(80A1)

A file in which CRYSTIN commands, such as BASE=1, ELC=1, etc., are written in order to classify substances in ICSD (CRYSTMET).

##### **3.2.2 ITOH4XC.@DATANO.DATA**

(2F5.2) (the first record)

(3(I5, A19))

A file in which the numerical values *DIFF1*, *DIFF2*, and the number of data (was confirmed in 3.1) are written.

#### **3.3 Output File**

##### **3.3.1 ITOH1XX.@SPG0.DATA**

A file which has ICSD (CRYSTMET) data.

##### **3.3.2 ITOH1XX.@SPGRP1.DATA**

A file which has ICSD (CRYSTMET) data transformed into EBCDIK code from 3.3.1.

##### **3.3.3 ITOH1XX.@SPGRP2.DATA**

A file which has the result of sorting inorganic species (collection code of ICSD (CRYSTMET))

##### **3.3.4 PRINT OUT, ITOH1XX.@SPGRP3.DATA**

Distribution of point groups

#### **3.4 Execution**

##### **3.4.1 CLIST**

ITOH4XC.MACRO.CLIST (ICSDMET)

#ITOH4XC.@ICSD.LOAD(ICSD) in the following lines is the FORTRAN program, produced by Gmelin-Institut für Anorganische Chemie and Fachinformationszentrum FIZ Karlsruhe, to search the ICSD or CRYSTMET databases.

```

/* EXHIBIT JOB MENU */
START:WRITE *** JOB MENU ***
WRITE 1. ICSD(INORGANIC CRYSTAL STRUCTURE DATABASE)
WRITE 2. CRYSTMET(THE NRCC METALS CRYSTALLOGRAPHIC DATA FILE)
WRITENR ENTER NUMBER =
READ &NUM
IF &NUM EQ 1 THEN GOTO ICSD
IF &NUM EQ 2 THEN GOTO CRYSTMET
WRITE ERROR &NUM
GOTO START
/* FILE SETTING FOR ICSD */
ICSD:ALLOC DD(FT40F001) DS(#ITOH1XX.&SPGO.DATA),REU
ALLOC DD(FT01F001) DS(#ITOH4XC.&ICSD.DATA),REU
ALLOC DD(FT02F001) DS(#ITOH4XC.&INDEX.FILE),REU
ALLOC DD(FT03F001) DS(#ITOH4XC.&TABLES.FILE),REU
GOTO EXICSD
END
/* FILE SETTING FOR CRYSTMET */
CRYSTMET:ALLOC DD(FT40F001) DS(#ITOH1XX.&SPGO.DATA),REU
ALLOC DD(FT01F001) DS(#ITOHXXX.&CRMET.DATA),REU
ALLOC DD(FT02F001) DS(#ITOHXXX.&INDEX.FILE),REU
ALLOC DD(FT03F001) DS(#ITOHXXX.&TABLES.FILE),REU
GOTO EXICSD
END
/* EXECUTE ICSD */
EXICSD:ALLOC DD(FT05F001) DS(#ITOH4XC.&COMMAND.DATA),REU
ALLOC DD(FT10F001) TE(AAA) SP(10,5) TR,REU
ALLOC DD(FT11F001) SY(E),CHARS(GC10),REU
CODE C
CALL #ITOH4XC.&ICSD.LOAD(ICSD)
ALLOC DD(FT05F001) DS(*),REU
ALLOC DD(FT06F001) DS(*),REU
FREE ALL
SUB #ITOH4XC.A.CNTL(ICSDMET)

```

### 3.4.2 JCL

ITOH4XC.A.CNTL(ICSDMET)

```

//XXXXXXXXB JOB *****,NOTIFY=XXXXXX,CLASS=C,MSGCLASS=C,
// REGION=(,128M)
//FLG EXEC FLG,PARAM=NOSOURCE
//FORT.SYSIN DD DSN=#ITOH4XC.SGRL.FORT(CHARCNV3),DISP=SHR
//GO.FT10F001 DD DSN=#ITOH1XX.&SPGO.DATA,DISP=SHR
//GO.FT11F001 DD DSN=#ITOH1XX.&SPGRP1.DATA,DISP=OLD
//FT06F001 DD SYSOUT=*
//FLG EXEC FLG,PARAM=NOSOURCE
//FORT.SYSIN DD DSN=#ITOH4XC.SGRL.FORT(INORDEF4),DISP=SHR
//GO.FT10F001 DD DSN=#ITOH1XX.&SPGRP1.DATA,DISP=SHR

```

```
//GO.FT11F001 DD DSN=#ITOH1XX.0SPGRP2.DATA,DISP=OLD
//GO.FT12F001 DD DSN=#ITOH4XC.0DATANO.DATA,DISP=SHR
//FT06F001 DD SYSOUT=*
//FLG EXEC FLG,PARAM=NOSOURCE
//FORT.SYSIN DD DSN=#ITOH4XC.SGRL.FORT(SGRDIST4),DISP=SHR
//GO.FT09F001 DD DSN=#ITOH1XX.0SPGRP2.DATA,DISP=SHR
//GO.FT10F001 DD DSN=#ITOH1XX.0SPGRP1.DATA,DISP=SHR
//GO.FT11F001 DD DSN=#ITOH1XX.0SPGRP3.DATA,DISP=OLD
//GO.FT12F001 DD DSN=#ITOH4XC.0DATANO.DATA,DISP=SHR
//
```

## 4 Examples

We study the statistical distribution of point groups for ICSD by the classification of the following categories, and also for CRYSTMET by the same categories except 4.3 ANX symbol. We give the result for ICSD.

- 1.ELEMENTS
- 2.CRYSTAL FAMILY
- 3.ANX SYMBOL

### 4.1 ELEMENTS

We define ‘Elements’ as a species whose chemical formula has one chemical element. We use the ICSD command ‘FIND ELC=1’. ELC is defined as ‘Number of different chemical elements’. Following the User’s manual, take Elements from ICSD, and count the number of substances (User’s manual 3.1). We obtain 218 substances by this command.

#### 4.1.1 Operation

The procedure is as follows.

```
>>EX #ITOH4XC.MACRO.CLIST(ICSD)(return)

*****      Crystal Structure Information System
* CRYSTIN *  (Release 2.51/Mar 90)
*****      Written by Hundt & Sievers (University of Bonn)

DB2201 - Please give BASE (or HELP) command.
Command?
BASE 1(return)
Command?
FIND ELC=1(return)
Current subset ("LAST") contains    218 entries.
Command?
QUIT(return)
>>
```

Type ‘BASE 1’ at first. The command to finish ICSD is ‘QUIT’.

For our study we edit following two files by ASPEN (User’s manual 3.2).

ITOH4XC.@COMMAND.DATA (80A1) (User’s manual 3.2.1)

```
>>ASP #ITOH4XC.QCOMMAND.DATA(return)

-----1-----2-----3-----4-----5-----6---
BASE 1
FIND ELC=1
PRINT 40 MINR,NAME,FORM,SGR,CELL
QUIT
```

Press PF11 (Save and End) to close the file.

ITOH4XC.@DATANO.DATA (2F5.2)(*DIFF1*, *DIFF2*)  
(3(I5, A18, 1X)) (numbers of data) (User's manual 3.2.2)

>>ASP #ITOH4XC.@DATANO.DATA(return)

-----1-----2-----3-----4-----5-----6--  
0.75 0.05  
218ELEMENT(ELC=1)

Press PF11 (Save and End) to close the file.

Execute ITOH4XC.MACRO.CLIST(ICSDMET). (User's manual 3.4.1)

>>EX #ITOH4XC.MACRO.CLIST(ICSDMET)(return)

\*\*\* JOB MENU \*\*\*

1. ICSD(INORGANIC CRYSTAL STRUCTURE DATABASE)
  2. CRYSTMET(THE NRCC METALS CRYSTALLOGRAPHIC DATA FILE)
- ENTER NUMBER =1(return)

\*\*\*\*\* Crystal Structure Information System  
\* CRYSTIN \* (Release 2.51/Mar 90)  
\*\*\*\*\* Written by Hundt & Sievers (University of Bonn)  
DB2201 - Please give BASE (or HELP) command.  
Command?  
Command?  
Current subset ("LAST") contains 218 entries.  
Command?  
Command?  
JOB ITOH4XCB(J Q26950) SUBMITTED  
>>

We obtain the statistical distribution of point groups for Elements. Output files and print out, which are in User's manual 3.3.1, are as follows.

#### 4.1.2 Data

Output file from ICSD (ITOH1XX.@SPG0.DATA) (User's manual 3.3.1)  
This file has Elements from ICSD.

```
0000      870      576  2 3 2 3
100    SULFUR
400    S
800    10.92600   2.E-3 10.85500   2.E-3 10.79000   3.E-3 90.000  -1.E 0
810    95.920    2.E-2 90.000  -1.E 0 64 2.010  -1.E 00.12729E+04
900    P121/C1
9900     870      576
0000      972      669  2 4 2 4
100    BORON - \-beta
400    B314.7
800    10.92510   2.E-4 10.92510   2.E-4 23.81429   8.E-4 90.000  -1.E 0
810    90.000  -1.E 0120.000  -1.E 0 1-1.000  -1.E 00.24617E+04
900    R3-MH
9900     972      669
0000      1402     1070  2 2 4 4
100    cyclo-Heptasulfur
400    S7
800    15.10500   5.E-3 5.99800   7.E-3 15.09600   5.E-3 90.000  -1.E 0
810    92.150    5.E-2 90.000  -1.E 0 8-1.000  -1.E 00.13667E+04
900    P121/N1
9900     1402     1070
```

Now we explain about the records.

```
<0000> Column
 1-8  ' 0000  ' Record label
 9-14 Collection code
 15  free
 16-20 Relative entry number
 22-80 free
< 100>,< 400>,< 900>
 1  free
 2-3  ' 1' Compound name
       ' 4' Chemical formula
       ' 9' Space group symbol after Hermann-Mauguin
 4  0
 5  Number of continuation records. 0 if the text contains
 less than 73 characters.
 6-8  free
 9-80 Text. After each 72 chacters a continuation record is
 used.
< 800>
 1-8  ' 800  ' Record label
 9-17 a(A)
```

18-25 Sigma(a)  
 26-34 b(A)  
 35-42 Sigma(b)  
 43-51 c(A)  
 52-59 Sigma(c)  
 60-66 Alpha(degrees)  
 67-74 Sigma(alpha)  
 75-80 free  
 < 810>  
 1-8 ' 810 ' Record label  
 9-15 Beta(degrees)  
 16-23 Sigma(beta)  
 24-30 Gamma(degrees)  
 31-38 Sigma(gamma)  
 39-41 Number of formula units  
 42-47 Measured density  
 48-55 Sigma(density)  
 55-66 Unit cell volume (A\*\*3)  
 56-80 free

Take the first substance (SULFUR) as an example.

\*First record

0000	RECORD LABEL
870	COLLECTION CODE
576	RELATIVE ENTRY NUMBER

\*Second record

100	RECORD LABEL
SULFUR	COMPOUND NAME

\*Third record

400	RECORD LABEL
S	CHEMICAL FORMULA

\*Fourth record

800	RECORD LABEL
10.92600	a(ANGSTROM)
2.E-3	SIGMA(a)=2.0*(10**(-3))
10.85500	b(ANGSTROM)
2.E-3	SIGMA(b)=2.0*(10**(-3))
10.79000	c(ANGSTROM)
3.E-3	SIGMA(c)=3.0*(10**(-3))
90.000	alpha(DEGREES)
-1.E 0	SIGMA(alpha)=0

\*Fifth record

810	RECORD LABEL
95.920	beta(DEGREES)
2.E-2	SIGMA(beta)=2.0*(10**(-2))

90.000	gamma(DEGREES)
-1.E 0	SIGMA(gamma)=0
64	Z
2.010	density(measured)
-1.E 0	SIGMA(density)=0
0.12729E+0.4	unit cell volume(ANGSTROM**3)=0.12729*(10**4)

\*Sixth record

900	RECORD LABEL
P121/C1	HERMANN-MAUGUIN SYMBOL

\*Seventh record

9900	RECORD LABEL
870	COLLECTION CODE
576	RELATIVE ENTRY NUMBER

The small letters of ITOH1XX.@SPG0.DATA are transformed into capital letters, and Hermann-Mauguin symbols are transformed into Schoenflies symbols. (ITOH1XX.@SPGRP1.DATA) (User's manual 3.3.2)

#### 4.1.3 Results

We define the species (representatives) of ELEMENTS (ITOH1XX.@SPGRP2.DATA) (User's manual 3.3.3). We consider that the number just after a serial number is a collection code of ICSD as a representative substance. The numbers of its rightside are concluded to be close to the representative. By using the ratio of the differences (*DIFF2*) of two primitive unit cell volumes, we obtain the statistical distribution of point groups. (cf. 2 Algorithm)

*DIFF2* : 0.025

1	870				
2	972	14288	18318		
3	1402	16470			
4	1418				
5	1425				
6	1637	36333			
7	2091				
8	2284				
9	2513				
10	2718	24635	24670	30606	
11	2795				
12	6002				
13	9140				
14	9745				
15	9777				
16	9785				
17	9786				
18	9859				
19	10083	15318	20329	24009	
20	10084				
21	12173				
22	12174				
23	15472	26482	28179		
24	15535				
25	15766	31458			
26	15767				
27	15819	27249			
28	15821	16573			
29	16056	16057	16058		
30	16262				
31	16386				
32	16469				
33	16516	16517	16518		
34	16569	16955			
35	16570	16954			
36	16574	21107			
37	18154	24653	201697	201698	201699
38	18311	31163			
39	20351				
40	20502				
41	20686				

42 20710  
43 22251  
44 22271  
45 22300 26636  
46 22384  
47 22406 27984 30318  
48 22410  
49 23058 23059 23060 23061  
50 23062 23063 23064 23065 23066 23067  
51 23068 23069 200685 200686  
52 23070 23071 23072 200687  
53 23073  
54 23074  
55 23075  
56 23247  
57 23836 27847 36432 36433 36434 36435 36436 36437 36438  
58 23914  
59 24019  
60 24602  
61 24622  
62 24787  
63 24788  
64 24891  
65 24892 31538  
66 24893  
67 26463  
68 26487 62747  
69 27261 27840 38147 200453 200454 200455  
70 27422  
71 27495 29071 37090  
72 28140 28141 28142 28143 28144  
73 28338  
74 28339 28464  
75 28340  
76 28344 62011 62012  
77 28465  
78 28466  
79 28539  
80 28540  
81 28856  
82 28857 28858 28859 28860 28861 28862 28863 29068 29151 29324  
29325  
83 29123  
84 29273  
85 29279  
86 29287 29288 60385 60386 60387 60388 60389  
87 30101  
88 31170  
89 31526

90 31532  
91 31540  
92 31684  
93 31692  
94 31829  
95 33693  
96 35186 61704  
97 36439 36440 36441 36442  
98 37059  
99 37238  
100 38263  
101 38264  
102 47169  
103 201692 201693 201694  
104 201695  
105 201696  
106 61539  
107 61541  
108 60650  
109 61705  
110 62003 62004 62005 62006 62007  
111 62008 62009 62010  
112 62013  
113 62014 62015  
114 62016  
115 62017  
116 62018  
117 62019 62020 62021  
118 62022  
119 62023

Consequently, the 218 crystalline substances have 119 representatives (species).

*DIFF2* : 0.050

1	870	1402	16470
2	972	14288	18318
3	1418		
4	1425		
5	1637	36333	
6	2091		
7	2284		
8	2513		
9	2718	24635	24670
10	2795		30606
11	6002		
12	9140		
13	9745		
14	9777		
15	9785		
16	9786		
17	9859		
18	10083	15318	20329
19	10084		24009
20	12173		
21	12174		
22	15472	26482	28179
23	15535		
24	15766	31458	
25	15767		
26	15819	27249	
27	15821	16573	
28	16056	16057	16058
29	16262		
30	16386		
31	16469		
32	16516	16517	16518
33	16569	16955	
34	16570	16954	
35	16574	21107	
36	18154	24653	201696
37	18311	201697	201698
38	20351	201699	
39	20502		
40	20686		
41	20710		
42	22251		
43	22271		
44	22300	26636	
45	22384		
46	22406	27984	30318
47	22410		
48	23058	23059	23060
		23061	23062
		23063	23064
		23065	23066
		23067	

49	23068	23069	23070	23071	200685	200686	200687			
50	23072	23073								
51	23074									
52	23075									
53	23247									
54	23836	27847	36432	36433	36434	36435	36436	36437	36438	36439
			36440	36441	36442					
55	23914									
56	24019									
57	24602	24787								
58	24622									
59	24788	29279								
60	24891									
61	24892	31538								
62	24893									
63	26463									
64	26487	62747								
65	27261	27840	38147	200453	200454	200455				
66	27422									
67	27495	29071	37090							
68	28140	28141	28142	28143	28144					
69	28338									
70	28339	28464								
71	28340									
72	28344	62009	62010	62011	62012					
73	28465									
74	28466									
75	28539									
76	28540									
77	28856									
78	28857	28858	28859	28860	28861	28862	28863	29068	29151	29324
		29325								
79	29123									
80	29273									
81	29287	29288	60385	60386	60387	60388	60389			
82	30101									
83	31170									
84	31526									
85	31532									
86	31540									
87	31684									
88	31692									
89	31829									
90	33693									
91	35186	61704								
92	37059									
93	37238									
94	38263									
95	38264									

96 47169  
97201692 201693 201694 201695  
98 61539  
99 61541  
100 60650  
101 61705  
102 62003 62004 62005 62006 62007 62008  
103 62013  
104 62014 62015 62016  
105 62017 62018  
106 62019 62020 62021 62022  
107 62023

Thus the 218 crystalline substances have 107 representatives (species).

Result1. Distribution of space groups and point groups. (ITOH4XC. @SPGRP3.DATA)  
(User's manual 3.3.4)

*DIFF2* : 0.025

ELEMENT(ELC=1) 0.025

C1 -1									
0									
CI -1									
0									
C2 -1	C2 -2	C2 -3							
1	1	1							
CS -1	CS -2	CS -3	CS -4						
0	0	0	0						
C2H-1	C2H-2	C2H-3	C2H-4	C2H-5	C2H-6				
0	1	3	2	7	4				
D2 -1	D2 -2	D2 -3	D2 -4	D2 -5	D2 -6	D2 -7	D2 -8	D2 -9	
0	0	0	1	0	0	0	0	0	
C2V-1	C2V-2	C2V-3	C2V-4	C2V-5	C2V-6	C2V-7	C2V-8	C2V-9	C2V-10
0	1	0	0	1	0	0	0	0	0
C2V-11	C2V-12	C2V-13	C2V-14	C2V-15	C2V-16	C2V-17	C2V-18	C2V-19	C2V-20
0	0	0	0	0	0	0	0	0	0
C2V-21	C2V-22								
0	0								
D2H-1	D2H-2	D2H-3	D2H-4	D2H-5	D2H-6	D2H-7	D2H-8	D2H-9	D2H-10
0	0	0	0	0	0	0	0	0	0
D2H-11	D2H-12	D2H-13	D2H-14	D2H-15	D2H-16	D2H-17	D2H-18	D2H-19	D2H-20
0	1	0	1	0	0	2	9	0	0
D2H-21	D2H-22	D2H-23	D2H-24	D2H-25	D2H-26	D2H-27	D2H-28		
0	0	1	1	0	0	0	0		
C4 -1	C4 -2	C4 -3	C4 -4	C4 -5	C4 -6				
0	0	0	1	1	0				
S4 -1	S4 -2								
0	0								
C4H-1	C4H-2	C4H-3	C4H-4	C4H-5	C4H-6				
0	0	0	0	2	0				
D4 -1	D4 -2	D4 -3	D4 -4	D4 -5	D4 -6	D4 -7	D4 -8	D4 -9	D4 -10
0	0	0	0	0	0	0	1	0	0
C4V-1	C4V-2	C4V-3	C4V-4	C4V-5	C4V-6	C4V-7	C4V-8	C4V-9	C4V-10
0	0	0	1	0	0	0	0	0	0
C4V-11	C4V-12								
0	0								
D2D-1	D2D-2	D2D-3	D2D-4	D2D-5	D2D-6	D2D-7	D2D-8	D2D-9	D2D-10
0	0	0	0	0	0	0	1	0	0
D2D-11	D2D-12								
0	0								
D4H-1	D4H-2	D4H-3	D4H-4	D4H-5	D4H-6	D4H-7	D4H-8	D4H-9	D4H-10
0	0	0	0	0	0	0	0	0	0
D4H-11	D4H-12	D4H-13	D4H-14	D4H-15	D4H-16	D4H-17	D4H-18	D4H-19	D4H-20

0	1	0	1	0	1	1	1	0	0	0
C3 -1	C3 -2	C3 -3	C3 -4							
1	0	0	0							
C3I-1	C3I-2									
0	1									
D3 -1	D3 -2	D3 -3	D3 -4	D3 -5	D3 -6	D3 -7				
0	0	0	6	0	0	0				
C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6					
0	0	0	0	0	0					
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6					
0	0	1	0	9	0					
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6					
0	0	0	0	0	0					
C3H-1										
0										
C6H-1	C6H-2									
0	0									
D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6					
0	0	0	0	0	0					
C6V-1	C6V-2	C6V-3	C6V-4							
0	0	0	2							
D3H-1	D3H-2	D3H-3	D3H-4							
0	0	0	0							
D6H-1	D6H-2	D6H-3	D6H-4							
0	0	0	16							
T -1	T -2	T -3	T -4	T -5						
0	0	2	2	0						
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6	TH -7				
0	0	0	0	1	3	1				
O -1	O -2	O -3	O -4	O -5	O -6	O -7	O -8	O -9	O -10	
0	0	3	0	10	0	2	0	0	0	
TD -1	TD -2	TD -3	TD -4	TD -5	TD -6					
0	0	0	0	0	1					
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6	OH -7	OH -8	OH -9	OH -10	
0	0	3	0	10	0	2	0	0	0	
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H
0	0	3	0	17	1	2	15	2	0	2
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H
1	1	1	4	1	1	6	0	10	0	0
C6H	D6	C6V	D3H	D6H	T	TH	0	TD	OH	TOTAL
0	0	2	0	16	4	5	0	1	15	110
<b>TOTAL=</b>										
0	0	3	0	17	1	2	15	2	0	2
1	1	1	4	1	1	6	0	10	0	0
0	0	2	0	16	4	5	0	1	15	110

Result2. Distribution of point groups. (PRINT OUT) (User's manual 3.3.4)

C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H
C6H	D6	C6V	D3H	D6H	T	TH	O	TD	OH	TOTAL
<b>DIFF2:0.025</b>										
0	0	3	0	17	1	2	15	2	0	2
1	1	1	4	1	1	6	0	10	0	0
0	0	2	0	16	4	5	0	1	15	110
<b>DIFF2:0.05</b>										
0	0	3	0	16	1	2	12	2	0	2
1	1	1	4	1	1	4	0	10	0	0
0	0	2	0	12	4	5	0	1	13	98
<b>DIFF2:0.075</b>										
0	0	3	0	16	1	2	12	2	0	2
1	1	1	4	1	1	3	0	9	0	0
0	0	2	0	10	3	5	0	1	13	93
<b>DIFF2:0.10</b>										
0	0	3	0	16	1	2	12	2	0	2
1	1	1	4	1	1	3	0	9	0	0
0	0	2	0	9	3	5	0	1	12	91
<b>DIFF2:0.125</b>										
0	0	3	0	16	1	2	12	2	0	2
1	1	1	4	1	1	3	0	9	0	0
0	0	2	0	7	3	5	0	1	12	89
<b>DIFF2:0.15</b>										
0	0	3	0	15	1	2	12	2	0	2
1	1	1	4	1	1	2	0	9	0	0
0	0	2	0	7	3	5	0	1	12	87
<b>DIFF2:0.175</b>										
0	0	3	0	15	1	2	12	2	0	2
1	1	1	4	1	1	2	0	9	0	0
0	0	2	0	6	3	5	0	1	12	86
<b>DIFF2:0.20</b>										
0	0	3	0	15	1	2	12	2	0	2
1	1	1	4	1	1	2	0	8	0	0
0	0	2	0	6	3	5	0	1	12	85
<b>DIFF2:0.225</b>										
0	0	3	0	14	1	2	12	2	0	2
1	1	1	4	1	1	2	0	8	0	0
0	0	2	0	6	3	5	0	1	12	84
<b>DIFF2:0.25</b>										
0	0	3	0	14	1	2	11	2	0	2
1	1	1	4	1	1	2	0	8	0	0
0	0	2	0	6	3	5	0	1	12	83

The reasons why the total number is less than the number of defined species, are as follows. Firstly some substances have Hermann-Mauguin symbols which cannot be transformed into Shoenflies symbols. Secondly there are some crystalline substances which do not have Hermann-Mauguin symbols, in ICSD. We omit the substances without Hermann-Mauguin symbols hereafter.

## 4.2 CRYSTAL FAMILY

ICSD has the descriptor 'SYST='. This descriptor is to choose substances by means of CRYSTAL FAMILY. In ICSD, substances are classified into six CRYSTAL FAMILY such as TRI (Triclinic), MON (Monoclinic), ORT (Orthorhombic), TET (Tetragonal), HEX (Hexagonal) and CUB (Cubic). In each CRYSTAL FAMILY, we examine the distribution of point groups. The method is the same as that of 4.1 ELEMENTS. To count the number of the substances by CRYSTAL FAMILY, we use DISPLAY command of ICSD.

```
>>EX #ITOH4XC.MACRO.CLIST(ICSD)(return)

***** Crustal Structure Information System
* CRYSTIN * (Release 2.51/Mar 90)
***** Written by Hundt & Sievers (University of Bonn)

DB2201 - Please give BASE (or HELP) command.
Command?
BASE 1(return)
Command?
DISPLAY SYST=(return)
L=001 Base 1: 4479 * SYST=CUB
L=002 Base 1: 4743 * SYST=HEX
L=003 Base 1: 5862 * SYST=MON
L=004 Base 1: 5922 * SYST=ORT
L=005 Base 1: 3100 * SYST=TET
L=006 Base 1: 1416 * SYST=TRI
Command?
QUIT(return)
>>
```

We edit two files below, by using these data.

```
>>ASP #ITOH4XC.QCOMMAND.DATA(return)

-----1----+---2----+---3----+---4----+---5----+---6
BASE 1
FIND SYST=TRI
PRINT 40 MINR,NAME,FORM,SGR,CELL
QUIT
```

Press PF11 (Save and End) to close the file.

```
>>ASP #ITOH4XC.QDATANO.DATA(return)

-----1----+---2----+---3----+---4----+---5----+---6
1416SYST=TRI          0
```

Press PF11 (Save and End) to close the file.

Edit above two files for each CRYSTAL FAMILY, then execute ITOH4XC.MACRO.CLIST(ICSDMET), we obtain the result.

>>EX #ITOH4XC.MACRO.CLIST(ICSDMET)(return)

*DIFF2* : 0.025

SYST=CUB

C1 -1										
0										
CI -1										
0										
C2 -1	C2 -2	C2 -3								
0	0	0								
CS -1	CS -2	CS -3	CS -4							
0	0	0	0							
C2H-1	C2H-2	C2H-3	C2H-4	C2H-5	C2H-6					
0	0	0	0	0	0					
D2 -1	D2 -2	D2 -3	D2 -4	D2 -5	D2 -6	D2 -7	D2 -8	D2 -9		
0	0	0	0	0	0	0	0	0		
C2V-1	C2V-2	C2V-3	C2V-4	C2V-5	C2V-6	C2V-7	C2V-8	C2V-9	C2V-10	
0	0	0	0	0	0	0	0	0	0	
C2V-11	C2V-12	C2V-13	C2V-14	C2V-15	C2V-16	C2V-17	C2V-18	C2V-19	C2V-20	
0	0	0	0	0	0	0	0	0	0	
C2V-21	C2V-22									
0	0									
D2H-1	D2H-2	D2H-3	D2H-4	D2H-5	D2H-6	D2H-7	D2H-8	D2H-9	D2H-10	
0	0	0	0	0	0	0	0	0	0	
D2H-11	D2H-12	D2H-13	D2H-14	D2H-15	D2H-16	D2H-17	D2H-18	D2H-19	D2H-20	
0	0	0	0	0	0	0	0	0	0	
D2H-21	D2H-22	D2H-23	D2H-24	D2H-25	D2H-26	D2H-27	D2H-28			
0	0	0	0	0	0	0	0			
C4 -1	C4 -2	C4 -3	C4 -4	C4 -5	C4 -6					
0	0	0	0	0	0					
S4 -1	S4 -2									
0	0									
C4H-1	C4H-2	C4H-3	C4H-4	C4H-5	C4H-6					
0	0	0	0	0	0					
D4 -1	D4 -2	D4 -3	D4 -4	D4 -5	D4 -6	D4 -7	D4 -8	D4 -9	D4 -10	
0	0	0	0	0	0	0	0	0	0	
C4V-1	C4V-2	C4V-3	C4V-4	C4V-5	C4V-6	C4V-7	C4V-8	C4V-9	C4V-10	
0	0	0	0	0	0	0	0	0	0	
C4V-11	C4V-12									
0	0									
D2D-1	D2D-2	D2D-3	D2D-4	D2D-5	D2D-6	D2D-7	D2D-8	D2D-9	D2D-10	
0	0	0	0	0	0	0	0	0	0	
D2D-11	D2D-12									
0	0									
D4H-1	D4H-2	D4H-3	D4H-4	D4H-5	D4H-6	D4H-7	D4H-8	D4H-9	D4H-10	

0	0	0	0	0	0	0	0	0	0	0	0
D4H-11	D4H-12	D4H-13	D4H-14	D4H-15	D4H-16	D4H-17	D4H-18	D4H-19	D4H-20		
0	0	0	0	0	0	0	0	0	0	0	0
C3 -1	C3 -2	C3 -3	C3 -4								
0	0	0	0								
C3I-1	C3I-2										
0	0										
D3 -1	D3 -2	D3 -3	D3 -4	D3 -5	D3 -6	D3 -7					
0	0	0	0	0	0	0					
C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6						
0	0	0	0	0	0						
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6						
0	0	0	0	0	0						
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6						
0	0	0	0	0	0						
C3H-1											
0											
C6H-1	C6H-2										
0	0										
D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6						
0	0	0	0	0	0						
C6V-1	C6V-2	C6V-3	C6V-4								
0	0	0	0								
D3H-1	D3H-2	D3H-3	D3H-4								
0	0	0	0								
D6H-1	D6H-2	D6H-3	D6H-4								
0	0	0	0								
T -1	T -2	T -3	T -4	T -5							
13	41	18	57	23							
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6	TH -7					
13	26	19	12	48	98	35					
O -1	O -2	O -3	O -4	O -5	O -6	O -7	O -8				
2	11	4	5	4	15	8	6				
TD -1	TD -2	TD -3	TD -4	TD -5	TD -6						
29	117	38	23	0	67						
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6	OH -7	OH -8	OH -9	OH -10		
200	2	26	14	533	10	297	9	37	76		
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
0	0	0	0	0	0	0	0	0	0	0	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
0	0	0	0	0	0	0	0	0	0	0	
C6H	D6	C6V	D3H	D6H	T	TH	0	TD	OH	TOTAL	
0	0	0	0	0	152	251	55	274	1204	1936	

SYST=HEX

C1 -1

	0										
CI	-1										
	0										
C2	-1	C2	-2	C2	-3						
	0	0	0	0	0						
CS	-1	CS	-2	CS	-3	CS	-4				
	0	0	0	0	0						
C2H	-1	C2H	-2	C2H	-3	C2H	-4	C2H	-5	C2H	-6
	0	0	0	0	0	0	0	0	0	0	
D2	-1	D2	-2	D2	-3	D2	-4	D2	-5	D2	-6
	0	0	0	0	0	0	0	0	0	0	
C2V	-1	C2V	-2	C2V	-3	C2V	-4	C2V	-5	C2V	-6
	0	0	0	0	0	0	0	0	0	0	
C2V	-11	C2V	-12	C2V	-13	C2V	-14	C2V	-15	C2V	-16
	0	0	0	0	0	0	0	0	0	0	
C2V	-21	C2V	-22								
	0	0									
D2H	-1	D2H	-2	D2H	-3	D2H	-4	D2H	-5	D2H	-6
	0	0	0	0	0	0	0	0	0	0	
D2H	-11	D2H	-12	D2H	-13	D2H	-14	D2H	-15	D2H	-16
	0	0	0	0	0	0	0	0	0	0	
D2H	-21	D2H	-22	D2H	-23	D2H	-24	D2H	-25	D2H	-26
	0	0	0	0	0	0	0	0	0	0	
C4	-1	C4	-2	C4	-3	C4	-4	C4	-5	C4	-6
	0	0	0	0	0	0	0	0	0	0	
S4	-1	S4	-2								
	0	0									
C4H	-1	C4H	-2	C4H	-3	C4H	-4	C4H	-5	C4H	-6
	0	0	0	0	0	0	0	0	0	0	
D4	-1	D4	-2	D4	-3	D4	-4	D4	-5	D4	-6
	0	0	0	0	0	0	0	0	0	0	
C4V	-1	C4V	-2	C4V	-3	C4V	-4	C4V	-5	C4V	-6
	0	0	0	0	0	0	0	0	0	0	
C4V	-11	C4V	-12								
	0	0									
D2D	-1	D2D	-2	D2D	-3	D2D	-4	D2D	-5	D2D	-6
	0	0	0	0	0	0	0	0	0	0	
D2D	-11	D2D	-12								
	0	0									
D4H	-1	D4H	-2	D4H	-3	D4H	-4	D4H	-5	D4H	-6
	0	0	0	0	0	0	0	0	0	0	
D4H	-11	D4H	-12	D4H	-13	D4H	-14	D4H	-15	D4H	-16
	0	0	0	0	0	0	0	0	0	0	
C3	-1	C3	-2	C3	-3	C3	-4				
	33	15	4	51							
C3I	-1	C3I	-2								
	41	244									
D3	-1	D3	-2	D3	-3	D3	-4	D3	-5	D3	-6
	11	47	6	37	1	7	41				

C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6						
47	15	4	19	136	47						
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6						
34	21	258	42	430	135						
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6						
1	6	1	1	0	66						
C3H-1											
27											
C6H-1	C6H-2										
5	146										
D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6						
4	2	0	20	4	26						
C6V-1	C6V-2	C6V-3	C6V-4								
0	1	25	120								
D3H-1	D3H-2	D3H-3	D3H-4								
29	14	59	24								
D6H-1	D6H-2	D6H-3	D6H-4								
89	11	46	361								
T -1	T -2	T -3	T -4	T -5							
0	0	0	0	0							
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6	TH -7					
0	0	0	0	0	0	0					
O -1	O -2	O -3	O -4	O -5	O -6	O -7	O -8	O -9	O -10		
0	0	0	0	0	0	0	0	0	0		
TD -1	TD -2	TD -3	TD -4	TD -5	TD -6						
0	0	0	0	0	0						
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6	OH -7	OH -8	OH -9	OH -10		
0	0	0	0	0	0	0	0	0	0		
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
0	0	0	0	0	0	0	0	0	0	0	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
0	0	0	0	103	285	150	268	920	75	27	
C6H	D6	C6V	D3H	D6H	T	TH	0	TD	OH	TOTAL	
151	56	146	126	507	0	0	0	0	0	2814	

SYST=MON

C1 -1											
0											
CI -1											
0											
C2 -1	C2 -2	C2 -3									
17	95	104									
CS -1	CS -2	CS -3	CS -4								
7	46	46	112								
C2H-1	C2H-2	C2H-3	C2H-4	C2H-5	C2H-6						
25	206	493	143	938	465						

D2 -1	D2 -2	D2 -3	D2 -4	D2 -5	D2 -6	D2 -7	D2 -8	D2 -9	
0	0	0	0	0	0	0	0	0	
C2V-1	C2V-2	C2V-3	C2V-4	C2V-5	C2V-6	C2V-7	C2V-8	C2V-9	C2V-10
0	0	0	0	0	0	0	0	0	0
C2V-11	C2V-12	C2V-13	C2V-14	C2V-15	C2V-16	C2V-17	C2V-18	C2V-19	C2V-20
0	0	0	0	0	0	0	0	0	0
C2V-21	C2V-22								
0	0								
D2H-1	D2H-2	D2H-3	D2H-4	D2H-5	D2H-6	D2H-7	D2H-8	D2H-9	D2H-10
0	0	0	0	0	0	0	0	0	0
D2H-11	D2H-12	D2H-13	D2H-14	D2H-15	D2H-16	D2H-17	D2H-18	D2H-19	D2H-20
0	0	0	0	0	0	0	0	0	0
D2H-21	D2H-22	D2H-23	D2H-24	D2H-25	D2H-26	D2H-27	D2H-28		
0	0	0	0	0	0	0	0		
C4 -1	C4 -2	C4 -3	C4 -4	C4 -5	C4 -6				
0	0	0	0	0	0				
S4 -1	S4 -2								
0	0								
C4H-1	C4H-2	C4H-3	C4H-4	C4H-5	C4H-6				
0	0	0	0	0	0				
D4 -1	D4 -2	D4 -3	D4 -4	D4 -5	D4 -6	D4 -7	D4 -8	D4 -9	D4 -10
0	0	0	0	0	0	0	0	0	0
C4V-1	C4V-2	C4V-3	C4V-4	C4V-5	C4V-6	C4V-7	C4V-8	C4V-9	C4V-10
0	0	0	0	0	0	0	0	0	0
C4V-11	C4V-12								
0	0								
D2D-1	D2D-2	D2D-3	D2D-4	D2D-5	D2D-6	D2D-7	D2D-8	D2D-9	D2D-10
0	0	0	0	0	0	0	0	0	0
D2D-11	D2D-12								
0	0								
D4H-1	D4H-2	D4H-3	D4H-4	D4H-5	D4H-6	D4H-7	D4H-8	D4H-9	D4H-10
0	0	0	0	0	0	0	0	0	0
D4H-11	D4H-12	D4H-13	D4H-14	D4H-15	D4H-16	D4H-17	D4H-18	D4H-19	D4H-20
0	0	0	0	0	0	0	0	0	0
C3 -1	C3 -2	C3 -3	C3 -4						
0	0	0	0						
C3I-1	C3I-2								
0	0								
D3 -1	D3 -2	D3 -3	D3 -4	D3 -5	D3 -6	D3 -7			
0	0	0	0	0	0	0			
C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6				
0	0	0	0	0	0				
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6				
0	0	0	0	0	0				
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6				
0	0	0	0	0	0				
C3H-1									
0									
C6H-1	C6H-2								

0	0										
D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6						
0	0	0	0	0	0						
C6V-1	C6V-2	C6V-3	C6V-4								
0	0	0	0								
D3H-1	D3H-2	D3H-3	D3H-4								
0	0	0	0								
D6H-1	D6H-2	D6H-3	D6H-4								
0	0	0	0								
T -1	T -2	T -3	T -4	T -5							
0	0	0	0	0							
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6	TH -7					
0	0	0	0	0	0	0					
O -1	O -2	O -3	O -4	O -5	O -6	O -7	O -8				
0	0	0	0	0	0	0	0				
TD -1	TD -2	TD -3	TD -4	TD -5	TD -6						
0	0	0	0	0	0						
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6	OH -7	OH -8	OH -9	OH -10		
0	0	0	0	0	0	0	0	0	0		
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
0	0	216	211	2270	0	0	0	0	0	0	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
0	0	0	0	0	0	0	0	0	0	0	
C6H	D6	C6V	D3H	D6H	T	TH	0	TD	OH	TOTAL	
0	0	0	0	0	0	0	0	0	0	2697	

SYST=ORT

C1 -1											
0											
CI -1											
0											
C2 -1	C2 -2	C2 -3									
0	0	0									
CS -1	CS -2	CS -3	CS -4								
0	0	0	0								
C2H-1	C2H-2	C2H-3	C2H-4	C2H-5	C2H-6						
0	0	0	0	0	0						
D2 -1	D2 -2	D2 -3	D2 -4	D2 -5	D2 -6	D2 -7	D2 -8	D2 -9			
8	4	31	171	34	11	4	5	1			
C2V-1	C2V-2	C2V-3	C2V-4	C2V-5	C2V-6	C2V-7	C2V-8	C2V-9	C2V-10		
10	28	0	7	55	5	60	16	182	16		
C2V-11	C2V-12	C2V-13	C2V-14	C2V-15	C2V-16	C2V-17	C2V-18	C2V-19	C2V-20		
8	120	3	25	8	19	19	7	57	19		
C2V-21	C2V-22										
1	19										
D2H-1	D2H-2	D2H-3	D2H-4	D2H-5	D2H-6	D2H-7	D2H-8	D2H-9	D2H-10		

	18	2	1	5	34	30	15	15	108	25
D2H-11	D2H-12	D2H-13	D2H-14	D2H-15	D2H-16	D2H-17	D2H-18	D2H-19	D2H-20	
64	109	79	127	177	950	262	90	44		12
D2H-21	D2H-22	D2H-23	D2H-24	D2H-25	D2H-26	D2H-27	D2H-28			
15	7	22	56	73	29	8	45			
C4 -1	C4 -2	C4 -3	C4 -4	C4 -5	C4 -6					
0	0	0	0	0	0					
S4 -1	S4 -2									
0	0									
C4H-1	C4H-2	C4H-3	C4H-4	C4H-5	C4H-6					
0	0	0	0	0	0					
D4 -1	D4 -2	D4 -3	D4 -4	D4 -5	D4 -6	D4 -7	D4 -8	D4 -9	D4 -10	
0	0	0	0	0	0	0	0	0	0	
C4V-1	C4V-2	C4V-3	C4V-4	C4V-5	C4V-6	C4V-7	C4V-8	C4V-9	C4V-10	
0	0	0	0	0	0	0	0	0	0	
C4V-11	C4V-12									
0	0									
D2D-1	D2D-2	D2D-3	D2D-4	D2D-5	D2D-6	D2D-7	D2D-8	D2D-9	D2D-10	
0	0	0	0	0	0	0	0	0	0	
D2D-11	D2D-12									
0	0									
D4H-1	D4H-2	D4H-3	D4H-4	D4H-5	D4H-6	D4H-7	D4H-8	D4H-9	D4H-10	
0	0	0	0	0	0	0	0	0	0	
D4H-11	D4H-12	D4H-13	D4H-14	D4H-15	D4H-16	D4H-17	D4H-18	D4H-19	D4H-20	
0	0	0	0	0	0	0	0	0	0	
C3 -1	C3 -2	C3 -3	C3 -4							
0	0	0	0							
C3I-1	C3I-2									
0	0									
D3 -1	D3 -2	D3 -3	D3 -4	D3 -5	D3 -6	D3 -7				
0	0	0	0	0	0	0				
C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6					
0	0	0	0	0	0					
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6					
0	0	0	0	0	0					
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6					
0	0	0	0	0	0					
C3H-1										
0										
C6H-1	C6H-2									
0	0									
D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6					
0	0	0	0	0	0					
C6V-1	C6V-2	C6V-3	C6V-4							
0	0	0	0							
D3H-1	D3H-2	D3H-3	D3H-4							
0	0	0	0							
D6H-1	D6H-2	D6H-3	D6H-4							
0	0	0	0							

T -1	T -2	T -3	T -4	T -5							
0	0	0	0	0							
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6	TH -7					
0	0	0	0	0	0	0					
O -1	O -2	O -3	O -4	O -5	O -6	O -7	O -8				
0	0	0	0	0	0	0	0				
TD -1	TD -2	TD -3	TD -4	TD -5	TD -6						
0	0	0	0	0	0						
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6	OH -7	OH -8	OH -9	OH -10		
0	0	0	0	0	0	0	0	0	0		
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
0	0	0	0	0	269	684	2422	0	0	0	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
0	0	0	0	0	0	0	0	0	0	0	
C6H	D6	C6V	D3H	D6H	T	TH	0	TD	OH	TOTAL	
0	0	0	0	0	0	0	0	0	0	3375	

SYST=TET

C1 -1											
0											
CI -1											
0											
C2 -1	C2 -2	C2 -3									
0	0	0									
CS -1	CS -2	CS -3	CS -4								
0	0	0	0								
C2H-1	C2H-2	C2H-3	C2H-4	C2H-5	C2H-6						
0	0	0	0	0	0						
D2 -1	D2 -2	D2 -3	D2 -4	D2 -5	D2 -6	D2 -7	D2 -8	D2 -9			
0	0	0	0	0	0	0	0	0			
C2V-1	C2V-2	C2V-3	C2V-4	C2V-5	C2V-6	C2V-7	C2V-8	C2V-9	C2V-10		
0	0	0	0	0	0	0	0	0	0		
C2V-11	C2V-12	C2V-13	C2V-14	C2V-15	C2V-16	C2V-17	C2V-18	C2V-19	C2V-20		
0	0	0	0	0	0	0	0	0	0		
C2V-21	C2V-22										
0	0										
D2H-1	D2H-2	D2H-3	D2H-4	D2H-5	D2H-6	D2H-7	D2H-8	D2H-9	D2H-10		
0	0	0	0	0	0	0	0	0	0		
D2H-11	D2H-12	D2H-13	D2H-14	D2H-15	D2H-16	D2H-17	D2H-18	D2H-19	D2H-20		
0	0	0	0	0	0	0	0	0	0		
D2H-21	D2H-22	D2H-23	D2H-24	D2H-25	D2H-26	D2H-27	D2H-28				
0	0	0	0	0	0	0	0				
C4 -1	C4 -2	C4 -3	C4 -4	C4 -5	C4 -6						
10	15	5	2	14	5						
S4 -1	S4 -2										
8	76										

C4H-1	C4H-2	C4H-3	C4H-4	C4H-5	C4H-6						
7	8	30	29	62	89						
D4 -1	D4 -2	D4 -3	D4 -4	D4 -5	D4 -6	D4 -7	D4 -8	D4 -9	D4 -10		
1	3	4	41	0	13	3	11	10	2		
C4V-1	C4V-2	C4V-3	C4V-4	C4V-5	C4V-6	C4V-7	C4V-8	C4V-9	C4V-10		
17	8	0	7	2	0	2	2	14	6		
C4V-11	C4V-12										
9	6										
D2D-1	D2D-2	D2D-3	D2D-4	D2D-5	D2D-6	D2D-7	D2D-8	D2D-9	D2D-10		
14	2	39	24	4	5	7	8	16	7		
D2D-11	D2D-12										
31	78										
D4H-1	D4H-2	D4H-3	D4H-4	D4H-5	D4H-6	D4H-7	D4H-8	D4H-9	D4H-10		
55	9	3	3	56	35	199	22	17	2		
D4H-11	D4H-12	D4H-13	D4H-14	D4H-15	D4H-16	D4H-17	D4H-18	D4H-19	D4H-20		
4	4	12	89	29	5	342	108	167	29		
C3 -1	C3 -2	C3 -3	C3 -4								
0	0	0	0								
C3I-1	C3I-2										
0	0										
D3 -1	D3 -2	D3 -3	D3 -4	D3 -5	D3 -6	D3 -7					
0	0	0	0	0	0	0					
C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6						
0	0	0	0	0	0						
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6						
0	0	0	0	0	0						
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6						
0	0	0	0	0	0						
C3H-1											
0											
C6H-1	C6H-2										
0	0										
D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6						
0	0	0	0	0	0						
C6V-1	C6V-2	C6V-3	C6V-4								
0	0	0	0								
D3H-1	D3H-2	D3H-3	D3H-4								
0	0	0	0								
D6H-1	D6H-2	D6H-3	D6H-4								
0	0	0	0								
T -1	T -2	T -3	T -4	T -5							
0	0	0	0	0							
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6	TH -7					
0	0	0	0	0	0	0					
O -1	O -2	O -3	O -4	O -5	O -6	O -7	O -8				
0	0	0	0	0	0	0	0				
TD -1	TD -2	TD -3	TD -4	TD -5	TD -6						
0	0	0	0	0	0						
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6	OH -7	OH -8	OH -9	OH -10		

0	0	0	0	0	0	0	0	0	0	0	0
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
0	0	0	0	0	0	0	0	51	84	225	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
88	73	235	1190	0	0	0	0	0	0	0	0
C6H	D6	C6V	D3H	D6H	T	TH	0	TD	OH	TOTAL	
0	0	0	0	0	0	0	0	0	0	1946	

SYST=TRI

C1 -1											
	80										
CI -1											
	466										
C2 -1	C2 -2	C2 -3									
	0	0	0								
CS -1	CS -2	CS -3	CS -4								
	0	0	0	0							
C2H-1	C2H-2	C2H-3	C2H-4	C2H-5	C2H-6						
	0	0	0	0	0						
D2 -1	D2 -2	D2 -3	D2 -4	D2 -5	D2 -6	D2 -7	D2 -8	D2 -9			
	0	0	0	0	0	0	0	0			
C2V-1	C2V-2	C2V-3	C2V-4	C2V-5	C2V-6	C2V-7	C2V-8	C2V-9	C2V-10		
	0	0	0	0	0	0	0	0	0		
C2V-11	C2V-12	C2V-13	C2V-14	C2V-15	C2V-16	C2V-17	C2V-18	C2V-19	C2V-20		
	0	0	0	0	0	0	0	0	0		
C2V-21	C2V-22										
	0	0									
D2H-1	D2H-2	D2H-3	D2H-4	D2H-5	D2H-6	D2H-7	D2H-8	D2H-9	D2H-10		
	0	0	0	0	0	0	0	0	0		
D2H-11	D2H-12	D2H-13	D2H-14	D2H-15	D2H-16	D2H-17	D2H-18	D2H-19	D2H-20		
	0	0	0	0	0	0	0	0	0		
D2H-21	D2H-22	D2H-23	D2H-24	D2H-25	D2H-26	D2H-27	D2H-28				
	0	0	0	0	0	0	0				
C4 -1	C4 -2	C4 -3	C4 -4	C4 -5	C4 -6						
	0	0	0	0	0						
S4 -1	S4 -2										
	0	0									
C4H-1	C4H-2	C4H-3	C4H-4	C4H-5	C4H-6						
	0	0	0	0	0						
D4 -1	D4 -2	D4 -3	D4 -4	D4 -5	D4 -6	D4 -7	D4 -8	D4 -9	D4 -10		
	0	0	0	0	0	0	0	0	0		
C4V-1	C4V-2	C4V-3	C4V-4	C4V-5	C4V-6	C4V-7	C4V-8	C4V-9	C4V-10		
	0	0	0	0	0	0	0	0	0		
C4V-11	C4V-12										
	0	0									
D2D-1	D2D-2	D2D-3	D2D-4	D2D-5	D2D-6	D2D-7	D2D-8	D2D-9	D2D-10		
	0	0									

0	0	0	0	0	0	0	0	0	0	0	0
D2D-11	D2D-12										
0	0										
D4H-1	D4H-2	D4H-3	D4H-4	D4H-5	D4H-6	D4H-7	D4H-8	D4H-9	D4H-10		
0	0	0	0	0	0	0	0	0	0	0	0
D4H-11	D4H-12	D4H-13	D4H-14	D4H-15	D4H-16	D4H-17	D4H-18	D4H-19	D4H-20		
0	0	0	0	0	0	0	0	0	0	0	0
C3 -1	C3 -2	C3 -3	C3 -4								
0	0	0	0								
C3I-1	C3I-2										
0	0										
D3 -1	D3 -2	D3 -3	D3 -4	D3 -5	D3 -6	D3 -7					
0	0	0	0	0	0	0					
C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6						
0	0	0	0	0	0						
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6						
0	0	0	0	0	0						
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6						
0	0	0	0	0	0						
C3H-1											
0											
C6H-1	C6H-2										
0	0										
D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6						
0	0	0	0	0	0						
C6V-1	C6V-2	C6V-3	C6V-4								
0	0	0	0								
D3H-1	D3H-2	D3H-3	D3H-4								
0	0	0	0								
D6H-1	D6H-2	D6H-3	D6H-4								
0	0	0	0								
T -1	T -2	T -3	T -4	T -5							
0	0	0	0	0							
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6	TH -7					
0	0	0	0	0	0	0					
O -1	O -2	O -3	O -4	O -5	O -6	O -7	O -8				
0	0	0	0	0	0	0	0				
TD -1	TD -2	TD -3	TD -4	TD -5	TD -6						
0	0	0	0	0	0						
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6	OH -7	OH -8	OH -9	OH -10		
0	0	0	0	0	0	0	0	0	0	0	0
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
80	466	0	0	0	0	0	0	0	0	0	0
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
0	0	0	0	0	0	0	0	0	0	0	0
C6H	D6	C6V	D3H	D6H	T	TH	0	TD	OH	TOTAL	
0	0	0	0	0	0	0	0	0	0	546	

TOTAL=											
80	466	216	211	2270	269	684	2422	51	84	225	
88	73	235	1190	103	285	150	268	920	75	27	
151	56	146	126	507	152	251	55	274	1204	13314	

DIFF2 : 0.025

SYST=CUB	4479	1936
SYST=HEX	4743	2815
SYST=MON	5862	2733
SYST=ORT	5922	3376
SYST=TET	3100	1946
SYST=TRI	1416	546

C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
C6H	D6	C6V	D3H	D6H	T	TH	O	TD	OH	TOTAL	
<b>SYST=CUB</b>											
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	152	251	55	274	1204	1936	
<b>SYST=HEX</b>											
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	103	285	150	268	920	75	27	
151	56	146	126	507	0	0	0	0	0	0	2814
<b>SYST=MON</b>											
0	0	216	211	2270	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	2697
<b>SYST=ORT</b>											
0	0	0	0	0	269	684	2422	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	3375
<b>SYST=TET</b>											
0	0	0	0	0	0	0	0	51	84	225	
88	73	235	1190	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1946
<b>SYST=TRI</b>											
80	466	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	546
<b>TOTAL=</b>											
80	466	216	211	2270	269	684	2422	51	84	225	
88	73	235	1190	103	285	150	268	920	75	27	
151	56	146	126	507	152	251	55	274	1204	13314	

Here, we change the ratio (DIFF2) from 0.025 to 0.15 by 0.025.

SYST=CUB											
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
C6H	D6	C6V	D3H	D6H	T	TH	O	TD	OH	TOTAL	
DIFF2:0.025											
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	152	251	55	274	1204	1936	
DIFF2:0.05											
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	151	236	54	261	1091	1793	
DIFF2:0.075											
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	147	233	54	255	1060	1749	
DIFF2:0.10											
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	147	232	54	254	1049	1736	
DIFF2:0.125											
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	145	232	54	251	1038	1720	
DIFF2:0.15											
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	144	232	54	250	1032	1712	
SYST=HEX											
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
C6H	D6	C6V	D3H	D6H	T	TH	O	TD	OH	TOTAL	
DIFF2:0.025											
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	103	285	150	268	920	75	27	
151	56	146	126	507	0	0	0	0	0	2814	
DIFF2:0.05											
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	99	273	135	249	865	71	27	
144	55	140	122	483	0	0	0	0	0	2663	
DIFF2:0.075											
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	98	270	133	239	833	68	27	
140	54	139	118	473	0	0	0	0	0	2592	
DIFF2:0.10											
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	95	266	131	232	812	67	27	
137	54	138	118	464	0	0	0	0	0	2541	

SYST=MON											
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
C6H	D6	C6V	D3H	D6H	T	TH	O	TD	OH	TOTAL	
DIFF2:0.125											
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	95	264	130	226	799	61	27	
134	54	136	118	459	0	0	0	0	0	2503	
DIFF2:0.15											
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	91	263	127	222	789	60	27	
140	54	134	118	455	0	0	0	0	0	2480	
SYST=ORT											
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
C6H	D6	C6V	D3H	D6H	T	TH	O	TD	OH	TOTAL	
DIFF2:0.025											
0	0	216	211	2270	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	2697	
DIFF2:0.05											
0	0	199	193	2042	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	2434	
DIFF2:0.075											
0	0	187	184	1921	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	2292	
DIFF2:0.10											
0	0	180	177	1841	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	2198	
DIFF2:0.125											
0	0	172	173	1766	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	2111	
DIFF2:0.15											
0	0	172	164	1724	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	2060	

0	0	0	0	0	0	0	0	0	0	0	3133
<b>DIFF2:0.075</b>											
0	0	0	0	0	236	608	2173	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	3017
<b>DIFF2:0.10</b>											
0	0	0	0	0	229	599	2127	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	2955
<b>DIFF2:0.125</b>											
0	0	0	0	0	228	588	2086	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	2902
<b>DIFF2:0.15</b>											
0	0	0	0	0	220	577	2048	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	2845
<b>SYST=TET</b>											
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
C6H	D6	C6V	D3H	D6H	T	TH	O	TD	OH	TOTAL	
<b>DIFF2:0.025</b>											
0	0	0	0	0	0	0	0	51	84	225	
88	73	235	1190	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1946
<b>DIFF2:0.05</b>											
0	0	0	0	0	0	0	0	50	82	217	
85	72	219	1142	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1867
<b>DIFF2:0.075</b>											
0	0	0	0	0	0	0	0	50	81	213	
83	72	216	1125	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1840
<b>DIFF2:0.10</b>											
0	0	0	0	0	0	0	0	50	77	211	
82	72	214	1113	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1819
<b>DIFF2:0.125</b>											
0	0	0	0	0	0	0	0	50	77	210	
81	72	213	1108	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1811
<b>DIFF2:0.15</b>											
0	0	0	0	0	0	0	0	50	76	210	
81	72	212	1099	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1800
<b>SYST=TRI</b>											
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	

D4 C6H	C4V D6	D2D C6V	D4H D3H	C3 D6H	C3I T	D3 TH	C3V O	D3D TD	C6 OH	C3H TOTAL
<b>DIFF2:0.025</b>										
80	466	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	546
<b>DIFF2:0.05</b>										
75	398	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	473
<b>DIFF2:0.075</b>										
73	369	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	442
<b>DIFF2:0.10</b>										
73	348	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	421
<b>DIFF2:0.125</b>										
70	330	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	400
<b>DIFF2:0.15</b>										
68	328	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	396

### 4.3 ANX SYMBOL

ICSD has the descriptor 'ANX' (formula type). This descriptor is to describe a chemical structure roughly by its oxidation numbers of the chemical elements. (e.g. ANX=AX describes  $NaCl$ ,  $CaCl$ , and ANX=ABX<sub>3</sub> describes  $KNO_3$ ,  $CaTiO_3$  etc.) That is, alphabets A-M describe elements whose oxidation states are positive, X-Z, W, V, U, T, S describe elements whose oxidation states are negative, and N-R describe elements whose oxidation states are 0. Here, hydrogen and its isotopes, if their oxidation states are positive, are disregarded. If one element in the structure has some different oxidation states, ICSD uses different alphabetical letters respectively. Within a group, the chemical elements are arranged according to increasing indices.

Examples for the ANX symbol in ICSD are as follows.

$Ca_2SiO_4$	ANX=AB2X4
$CaSO_4(H_2O)_2$	ANX=ABX6
$(Na_{0.2}K_{0.8})(AlSi_3)O_8$	ANX=AB4X8
$NaTl$	ANX=NO
$H_2O$	ANX=X
$CaH_2$	ANX=AX2
$Na_2S_2O_3$	ANX=AB2XY3
$Fe_3O_4$	ANX=AB2X4

ICSD 1990 has 3775 ANX symbols. We study the statistical distributions of point groups for 34 ANX symbols, which have more than 100 substances in ICSD. To count the number of substances per ANX symbol, we use DISPLAY command of ICSD.

```
>>EX #ITOH4XC.MACRO.CLIST(ICSD)(return)

*****
      Crystal Structure Information System
* CRYSTIN *   (Release 2.51/Mar 90)
*****
      Written by Hundt & Sievers (University of Bonn)
DB2201 - Please give BASE (or HELP) command.

Command?
BASE 1
Command?
DISPLAY ANX=
L=001 Base 1: 215 * ANX=N
L=002 Base 1: 76 * ANX=X
L=003 Base 1: 913 * ANX=AX
L=004 Base 1: 7 * ANX=AX10
L=005 Base 1: 5 * ANX=AX12
L=006 Base 1: 13 * ANX=AX14
L=007 Base 1: 1 * ANX=AX15
L=008 Base 1: 1 * ANX=AX16
L=009 Base 1: 6 * ANX=AX18
L=010 Base 1: 1122 * ANX=AX2
L=011 Base 1: 3 * ANX=AX20
L=012 Base 1: 13 * ANX=AX22
L=013 Base 1: 3 * ANX=AX26
L=014 Base 1: 2 * ANX=AX28
```

... more (Y/N)?

N

Command?

QUIT

>>

We edit two files below, by using these data.

>>ASP #ITOH4XC.QCOMMAND.DATA(return)

-----+---1---+---2---+---3---+---4---+---5---+---6  
\*\* top of the data \*\*  
BASE 1  
FIND ANX=ABX3  
PRINT 40 MINR,NAME,FORM,SGR,CELL  
FIND ANX=AB2X4  
PRINT 40 MINR,NAME,FORM,SGR,CELL  
FIND ANX=AX2  
PRINT 40 MINR,NAME,FORM,SGR,CELL  
FIND ANX=AX  
PRINT 40 MINR,NAME,FORM,SGR,CELL  
FIND ANX=ABX4  
PRINT 40 MINR,NAME,FORM,SGR,CELL  
:  
FIND ANX=AXY2  
PRINT 40 MINR,NAME,FORM,SGR,CELL  
QUIT

Press PF11 (Save and End) to close the file.

>>ASP #ITOH4XC.QDATANO.DATA(return)

-----+---1---+---2---+---3---+---4---+---5---+---6  
\*\* top of the data \*\*  
1248ABX3 1131AB2X4 1122AX2  
913AX 816ABX4 666AB2X6  
499AX3 463ABX2 439ABC2X6  
345N02 333A2X3 300NO  
263AXY 233AB2X5 221A3X4  
215N 212A2B2X7 196ABX6  
166AB2X2 162NOP 154ABCX4  
150AB3X6 148AB2X3 143N02P2  
139A2B3C3X12 135ABX5 134A2B3X8  
133AX4 129AB2X8 123AB4X8  
112AB2X7 111N03 110ABX  
101AXY2 0

Press PF11 (Save and End) to close the file.

For ANX symbols, the distributions of point groups and space groups are as follows.  
 (ITOH1XX.@SPGRP3.DATA) (User's Manual 3.3.4)

*DIFF2 : 0.05*

ABX3

C1 -1																				
	3																			
CI -1																				
	15																			
C2 -1	C2 -2	C2 -3																		
	1	0	4																	
CS -1	CS -2	CS -3	CS -4																	
	2	2	2	4																
C2H-1	C2H-2	C2H-3	C2H-4	C2H-5	C2H-6															
	3	8	8	3	33	17														
D2 -1	D2 -2	D2 -3	D2 -4	D2 -5	D2 -6	D2 -7	D2 -8	D2 -9												
	0	0	0	8	3	0	0	0												
C2V-1	C2V-2	C2V-3	C2V-4	C2V-5	C2V-6	C2V-7	C2V-8	C2V-9	C2V-10											
	0	2	0	1	2	0	1	2	11											
C2V-11	C2V-12	C2V-13	C2V-14	C2V-15	C2V-16	C2V-17	C2V-18	C2V-19	C2V-20											
	0	2	0	2	0	0	0	0	0											
C2V-21	C2V-22																			
	0	0																		
D2H-1	D2H-2	D2H-3	D2H-4	D2H-5	D2H-6	D2H-7	D2H-8	D2H-9	D2H-10											
	3	0	0	0	1	1	0	0	0											
D2H-11	D2H-12	D2H-13	D2H-14	D2H-15	D2H-16	D2H-17	D2H-18	D2H-19	D2H-20											
	5	0	4	3	12	129	8	2	4											
D2H-21	D2H-22	D2H-23	D2H-24	D2H-25	D2H-26	D2H-27	D2H-28													
	0	0	0	3	3	0	0	1												
C4 -1	C4 -2	C4 -3	C4 -4	C4 -5	C4 -6															
	0	1	0	0	0															
S4 -1	S4 -2																			
	0	1																		
C4H-1	C4H-2	C4H-3	C4H-4	C4H-5	C4H-6															
	0	0	0	1	1	3														
D4 -1	D4 -2	D4 -3	D4 -4	D4 -5	D4 -6	D4 -7	D4 -8	D4 -9	D4 -10											
	0	0	0	0	0	0	0	0	0											
C4V-1	C4V-2	C4V-3	C4V-4	C4V-5	C4V-6	C4V-7	C4V-8	C4V-9	C4V-10											
	11	0	0	0	0	0	0	0	0											
C4V-11	C4V-12																			
	0	0																		
D2D-1	D2D-2	D2D-3	D2D-4	D2D-5	D2D-6	D2D-7	D2D-8	D2D-9	D2D-10											
	1	0	0	1	1	0	0	0	0											
D2D-11	D2D-12																			
	0	0																		
D4H-1	D4H-2	D4H-3	D4H-4	D4H-5	D4H-6	D4H-7	D4H-8	D4H-9	D4H-10											
	4	0	0	0	4	0	0	0	0											
D4H-11	D4H-12	D4H-13	D4H-14	D4H-15	D4H-16	D4H-17	D4H-18	D4H-19	D4H-20											

0	0	1	0	1	0	2	4	0	0	
C3 -1	C3 -2	C3 -3	C3 -4							
0	2	1	4							
C3I-1	C3I-2									
1	21									
D3 -1	D3 -2	D3 -3	D3 -4	D3 -5	D3 -6	D3 -7				
0	2	0	0	0	0	0				
C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6					
1	1	0	0	20	9					
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6					
0	1	0	1	17	23					
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6					
0	1	0	0	0	3					
C3H-1										
0										
C6H-1	C6H-2									
0	2									
D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6					
0	1	0	0	0	3					
C6V-1	C6V-2	C6V-3	C6V-4							
0	0	9	8							
D3H-1	D3H-2	D3H-3	D3H-4							
1	2	1	1							
D6H-1	D6H-2	D6H-3	D6H-4							
0	0	1	61							
T -1	T -2	T -3	T -4	T -5						
5	0	0	2	0						
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6	TH -7				
0	1	0	0	0	1	0				
O -1	O -2	O -3	O -4	O -5	O -6	O -7	O -8	O -9	O -10	
1	0	0	0	0	0	0	0	0	0	
TD -1	TD -2	TD -3	TD -4	TD -5	TD -6					
2	0	1	0	0	0					
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6	OH -7	OH -8	OH -9	OH -10	
98	0	0	0	5	0	7	0	0	0	
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H
3	15	5	10	72	11	23	179	1	1	5
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H
0	12	3	16	7	22	2	31	42	4	0
C6H	D6	C6V	D3H	D6H	T	TH	0	TD	OH	TOTAL
2	4	17	5	62	7	2	1	3	110	677

AB2X4

C1 -1  
2

CI -1									
	9								
C2 -1	C2 -2	C2 -3							
	0	7	1						
CS -1	CS -2	CS -3	CS -4						
	0	1	2	2					
C2H-1	C2H-2	C2H-3	C2H-4	C2H-5	C2H-6				
	1	6	14	2	25	6			
D2 -1	D2 -2	D2 -3	D2 -4	D2 -5	D2 -6	D2 -7	D2 -8	D2 -9	
	0	0	1	0	0	0	0	0	
C2V-1	C2V-2	C2V-3	C2V-4	C2V-5	C2V-6	C2V-7	C2V-8	C2V-9	C2V-10
	0	1	0	0	2	0	0	0	17
C2V-11	C2V-12	C2V-13	C2V-14	C2V-15	C2V-16	C2V-17	C2V-18	C2V-19	C2V-20
	0	1	0	0	0	0	2	0	2
C2V-21	C2V-22								
	0	0							
D2H-1	D2H-2	D2H-3	D2H-4	D2H-5	D2H-6	D2H-7	D2H-8	D2H-9	D2H-10
	0	0	0	0	2	2	0	0	8
D2H-11	D2H-12	D2H-13	D2H-14	D2H-15	D2H-16	D2H-17	D2H-18	D2H-19	D2H-20
	2	1	2	4	3	90	5	8	2
D2H-21	D2H-22	D2H-23	D2H-24	D2H-25	D2H-26	D2H-27	D2H-28		
	0	0	3	14	0	0	0	8	
C4 -1	C4 -2	C4 -3	C4 -4	C4 -5	C4 -6				
	0	0	0	0	1	0			
S4 -1	S4 -2								
	0	22							
C4H-1	C4H-2	C4H-3	C4H-4	C4H-5	C4H-6				
	0	0	0	0	5	2			
D4 -1	D4 -2	D4 -3	D4 -4	D4 -5	D4 -6	D4 -7	D4 -8	D4 -9	D4 -10
	0	0	1	0	0	0	1	0	0
C4V-1	C4V-2	C4V-3	C4V-4	C4V-5	C4V-6	C4V-7	C4V-8	C4V-9	C4V-10
	0	0	0	0	0	0	0	0	1
C4V-11	C4V-12								
	0	0							
D2D-1	D2D-2	D2D-3	D2D-4	D2D-5	D2D-6	D2D-7	D2D-8	D2D-9	D2D-10
	3	0	0	0	0	0	1	0	1
D2D-11	D2D-12								
	2	6							
D4H-1	D4H-2	D4H-3	D4H-4	D4H-5	D4H-6	D4H-7	D4H-8	D4H-9	D4H-10
	4	0	0	1	0	0	0	3	1
D4H-11	D4H-12	D4H-13	D4H-14	D4H-15	D4H-16	D4H-17	D4H-18	D4H-19	D4H-20
	0	0	4	0	0	0	36	7	11
C3 -1	C3 -2	C3 -3	C3 -4						
	0	0	0	0					
C3I-1	C3I-2								
	0	8							
D3 -1	D3 -2	D3 -3	D3 -4	D3 -5	D3 -6	D3 -7			
	0	0	1	0	0	0	0		
C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6				

0	0	0	0	1	1
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6
0	0	7	0	7	1
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6
0	0	0	0	0	3
C3H-1					
0					
C6H-1	C6H-2				
0	2				
D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6
0	0	0	0	0	3
C6V-1	C6V-2	C6V-3	C6V-4		
0	0	0	2		
D3H-1	D3H-2	D3H-3	D3H-4		
0	0	1	0		
D6H-1	D6H-2	D6H-3	D6H-4		
0	0	0	6		
T -1	T -2	T -3	T -4	T -5	
0	0	0	1	0	
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6
0	0	0	1	0	3
0 -1	0 -2	0 -3	0 -4	0 -5	0 -6
0	0	0	0	0	0
0 -7	0 -8				
TD -1	TD -2	TD -3	TD -4	TD -5	TD -6
0	4	0	0	0	0
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6
1	0	0	0	1	0
OH -7	OH -8	OH -9	OH -10		
				93	0

C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H
2	9	8	5	54	1	26	161	1	22	7
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H
2	1	13	68	0	8	1	2	15	3	0
C6H	D6	C6V	D3H	D6H	T	TH	0	TD	OH	TOTAL
2	3	2	1	6	1	4	0	4	95	527

## AX2

C1 -1										
3										
CI -1										
4										
C2 -1	C2 -2	C2 -3								
0	1	2								
CS -1	CS -2	CS -3	CS -4							
0	1	1	2							
C2H-1	C2H-2	C2H-3	C2H-4	C2H-5	C2H-6					
1	4	11	0	30	6					
D2 -1	D2 -2	D2 -3	D2 -4	D2 -5	D2 -6	D2 -7	D2 -8	D2 -9		

1	0	0	9	1	1	1	0	0	
C2V-1	C2V-2	C2V-3	C2V-4	C2V-5	C2V-6	C2V-7	C2V-8	C2V-9	C2V-10
0	0	0	0	1	0	3	0	5	0
C2V-11	C2V-12	C2V-13	C2V-14	C2V-15	C2V-16	C2V-17	C2V-18	C2V-19	C2V-20
0	8	0	0	0	1	1	0	1	1
C2V-21	C2V-22								
0	0								
D2H-1	D2H-2	D2H-3	D2H-4	D2H-5	D2H-6	D2H-7	D2H-8	D2H-9	D2H-10
0	0	0	0	0	0	0	0	0	0
D2H-11	D2H-12	D2H-13	D2H-14	D2H-15	D2H-16	D2H-17	D2H-18	D2H-19	D2H-20
0	14	1	8	11	30	5	3	0	0
D2H-21	D2H-22	D2H-23	D2H-24	D2H-25	D2H-26	D2H-27	D2H-28		
0	0	0	1	1	4	0	1		
C4 -1	C4 -2	C4 -3	C4 -4	C4 -5	C4 -6				
0	0	0	0	0	1				
S4 -1	S4 -2								
0	1								
C4H-1	C4H-2	C4H-3	C4H-4	C4H-5	C4H-6				
0	2	2	0	3	2				
D4 -1	D4 -2	D4 -3	D4 -4	D4 -5	D4 -6	D4 -7	D4 -8	D4 -9	D4 -10
0	0	0	5	0	10	0	3	0	0
C4V-1	C4V-2	C4V-3	C4V-4	C4V-5	C4V-6	C4V-7	C4V-8	C4V-9	C4V-10
0	0	0	0	0	0	0	0	0	0
C4V-11	C4V-12								
0	0								
D2D-1	D2D-2	D2D-3	D2D-4	D2D-5	D2D-6	D2D-7	D2D-8	D2D-9	D2D-10
1	0	2	0	0	0	0	0	0	0
D2D-11	D2D-12								
0	4								
D4H-1	D4H-2	D4H-3	D4H-4	D4H-5	D4H-6	D4H-7	D4H-8	D4H-9	D4H-10
2	0	0	0	0	0	9	0	0	0
D4H-11	D4H-12	D4H-13	D4H-14	D4H-15	D4H-16	D4H-17	D4H-18	D4H-19	D4H-20
0	0	1	34	3	0	14	3	6	4
C3 -1	C3 -2	C3 -3	C3 -4						
0	0	0	0						
C3I-1	C3I-2								
0	2								
D3 -1	D3 -2	D3 -3	D3 -4	D3 -5	D3 -6	D3 -7			
1	1	0	2	0	3	5			
C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6				
12	0	0	0	9	0				
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6				
1	0	29	1	19	0				
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6				
0	0	0	0	0	0				
C3H-1									
1									
C6H-1	C6H-2								
1	0								

D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6						
0	0	0	2	0	1						
C6V-1	C6V-2	C6V-3	C6V-4								
0	0	0	5								
D3H-1	D3H-2	D3H-3	D3H-4								
1	0	2	0								
D6H-1	D6H-2	D6H-3	D6H-4								
3	1	0	9								
T -1	T -2	T -3	T -4	T -5							
0	0	0	2	0							
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6	TH -7					
0	2	0	1	1	25	2					
O -1	O -2	O -3	O -4	O -5	O -6	O -7	O -8				
0	0	0	1	0	0	0	0				
TD -1	TD -2	TD -3	TD -4	TD -5	TD -6						
0	1	2	1	0	0						
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6	OH -7	OH -8	OH -9	OH -10		
0	0	0	0	64	0	4	0	1	0		

C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
3	4	3	4	52	13	21	79	1	1	9	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
18	0	7	76	0	2	12	21	50	0	1	
C6H	D6	C6V	D3H	D6H	T	TH	0	TD	OH	TOTAL	
1	3	5	3	13	2	31	1	4	69	509	

## AX

C1 -1											
0											
CI -1											
3											
C2 -1	C2 -2	C2 -3									
0	1	1									
CS -1	CS -2	CS -3	CS -4								
0	0	0	0								
C2H-1	C2H-2	C2H-3	C2H-4	C2H-5	C2H-6						
0	7	8	0	13	4						
D2 -1	D2 -2	D2 -3	D2 -4	D2 -5	D2 -6	D2 -7	D2 -8	D2 -9			
0	0	0	3	0	1	0	0	0			
C2V-1	C2V-2	C2V-3	C2V-4	C2V-5	C2V-6	C2V-7	C2V-8	C2V-9	C2V-10		
0	0	0	1	1	0	1	0	3	0		
C2V-11	C2V-12	C2V-13	C2V-14	C2V-15	C2V-16	C2V-17	C2V-18	C2V-19	C2V-20		
0	4	0	0	0	1	2	0	1	1		
C2V-21	C2V-22										
0	0										
D2H-1	D2H-2	D2H-3	D2H-4	D2H-5	D2H-6	D2H-7	D2H-8	D2H-9	D2H-10		
0	0	0	0	0	0	0	0	0	0		

D2H-11	D2H-12	D2H-13	D2H-14	D2H-15	D2H-16	D2H-17	D2H-18	D2H-19	D2H-20
1	2	1	1	1	23	13	1	0	0
D2H-21	D2H-22	D2H-23	D2H-24	D2H-25	D2H-26	D2H-27	D2H-28		
1	0	2	2	4	0	0	0		
C4 -1	C4 -2	C4 -3	C4 -4	C4 -5	C4 -6				
1	0	0	0	0	1				
S4 -1	S4 -2								
1	3								
C4H-1	C4H-2	C4H-3	C4H-4	C4H-5	C4H-6				
0	1	1	0	1	0				
D4 -1	D4 -2	D4 -3	D4 -4	D4 -5	D4 -6	D4 -7	D4 -8	D4 -9	D4 -10
0	0	0	0	0	0	0	0	0	0
C4V-1	C4V-2	C4V-3	C4V-4	C4V-5	C4V-6	C4V-7	C4V-8	C4V-9	C4V-10
0	0	0	0	0	0	0	0	0	0
C4V-11	C4V-12								
1	0								
D2D-1	D2D-2	D2D-3	D2D-4	D2D-5	D2D-6	D2D-7	D2D-8	D2D-9	D2D-10
0	0	0	0	0	0	1	1	1	0
D2D-11	D2D-12								
0	0								
D4H-1	D4H-2	D4H-3	D4H-4	D4H-5	D4H-6	D4H-7	D4H-8	D4H-9	D4H-10
0	0	0	0	0	0	8	0	4	0
D4H-11	D4H-12	D4H-13	D4H-14	D4H-15	D4H-16	D4H-17	D4H-18	D4H-19	D4H-20
0	0	0	4	1	2	8	0	3	2
C3 -1	C3 -2	C3 -3	C3 -4						
0	0	0	0						
C3I-1	C3I-2								
0	0								
D3 -1	D3 -2	D3 -3	D3 -4	D3 -5	D3 -6	D3 -7			
0	0	0	2	0	1	1			
C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6				
1	0	0	0	10	0				
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6				
0	0	5	0	18	0				
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6				
0	1	0	0	0	1				
C3H-1									
3									
C6H-1	C6H-2								
0	0								
D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6				
0	0	0	0	0	0				
C6V-1	C6V-2	C6V-3	C6V-4						
0	0	0	23						
D3H-1	D3H-2	D3H-3	D3H-4						
1	0	4	1						
D6H-1	D6H-2	D6H-3	D6H-4						
1	0	0	15						
T -1	T -2	T -3	T -4	T -5					

2	31	0	2	0							
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6	TH -7					
0	0	0	0	0	0	0					
0 -1	0 -2	0 -3	0 -4	0 -5	0 -6	0 -7	0 -8				
0	0	0	0	0	0	0	0				
TD -1	TD -2	TD -3	TD -4	TD -5	TD -6						
0	26	0	0	0	0						
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6	OH -7	OH -8	OH -9	OH -10		
26	0	0	0	126	0	2	0	9	1		
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
0	3	2	0	32	4	15	52	2	4	3	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
0	1	3	32	0	0	4	11	23	2	3	
C6H	D6	C6V	D3H	D6H	T	TH	0	TD	OH	TOTAL	
0	0	23	6	16	35	0	0	26	164	466	

#### ABX4

C1 -1											
2											
CI -1											
13											
C2 -1	C2 -2	C2 -3									
0	4	2									
CS -1	CS -2	CS -3	CS -4								
0	3	0	0								
C2H-1	C2H-2	C2H-3	C2H-4	C2H-5	C2H-6						
0	7	14	23	55	11						
D2 -1	D2 -2	D2 -3	D2 -4	D2 -5	D2 -6	D2 -7	D2 -8	D2 -9			
1	0	1	7	3	0	1	1	0			
C2V-1	C2V-2	C2V-3	C2V-4	C2V-5	C2V-6	C2V-7	C2V-8	C2V-9	C2V-10		
0	0	0	0	2	0	2	0	4	0		
C2V-11	C2V-12	C2V-13	C2V-14	C2V-15	C2V-16	C2V-17	C2V-18	C2V-19	C2V-20		
0	6	0	1	0	1	0	0	4	0		
C2V-21	C2V-22										
0	5										
D2H-1	D2H-2	D2H-3	D2H-4	D2H-5	D2H-6	D2H-7	D2H-8	D2H-9	D2H-10		
0	0	0	0	0	8	0	0	2	0		
D2H-11	D2H-12	D2H-13	D2H-14	D2H-15	D2H-16	D2H-17	D2H-18	D2H-19	D2H-20		
5	0	1	6	3	43	23	1	2	0		
D2H-21	D2H-22	D2H-23	D2H-24	D2H-25	D2H-26	D2H-27	D2H-28				
0	0	0	1	0	0	1	5				
C4 -1	C4 -2	C4 -3	C4 -4	C4 -5	C4 -6						
0	1	0	0	0	0						
S4 -1	S4 -2										
0	8										
C4H-1	C4H-2	C4H-3	C4H-4	C4H-5	C4H-6						

0	0	1	0	0	36					
D4 -1	D4 -2	D4 -3	D4 -4	D4 -5	D4 -6	D4 -7	D4 -8	D4 -9	D4 -10	
0	0	0	0	0	0	0	0	0	0	0
C4V-1	C4V-2	C4V-3	C4V-4	C4V-5	C4V-6	C4V-7	C4V-8	C4V-9	C4V-10	
0	0	0	0	0	0	0	0	0	0	0
C4V-11	C4V-12									
0	0									
D2D-1	D2D-2	D2D-3	D2D-4	D2D-5	D2D-6	D2D-7	D2D-8	D2D-9	D2D-10	
0	1	0	0	0	0	0	0	0	0	2
D2D-11	D2D-12									
1	5									
D4H-1	D4H-2	D4H-3	D4H-4	D4H-5	D4H-6	D4H-7	D4H-8	D4H-9	D4H-10	
3	0	0	0	2	0	3	0	0	0	0
D4H-11	D4H-12	D4H-13	D4H-14	D4H-15	D4H-16	D4H-17	D4H-18	D4H-19	D4H-20	
0	0	0	0	0	0	0	12	53	2	
C3 -1	C3 -2	C3 -3	C3 -4							
0	2	0	1							
C3I-1	C3I-2									
0	1									
D3 -1	D3 -2	D3 -3	D3 -4	D3 -5	D3 -6	D3 -7				
0	0	0	7	0	0	0				
C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6					
0	0	0	0	0	2					
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6					
0	0	0	0	7	0					
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6					
0	0	0	0	0	1					
C3H-1										
1										
C6H-1	C6H-2									
0	0									
D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6					
0	0	0	4	1	0					
C6V-1	C6V-2	C6V-3	C6V-4							
0	0	0	0							
D3H-1	D3H-2	D3H-3	D3H-4							
0	0	2	0							
D6H-1	D6H-2	D6H-3	D6H-4							
0	0	0	0							
T -1	T -2	T -3	T -4	T -5						
0	2	0	1	0						
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6	TH -7				
0	0	0	0	0	0	0				
O -1	O -2	O -3	O -4	O -5	O -6	O -7	O -8			
0	0	0	0	0	0	0	0			
TD -1	TD -2	TD -3	TD -4	TD -5	TD -6					
0	10	0	0	0	0					
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6	OH -7	OH -8	OH -9	OH -10	
1	0	0	0	9	0	2	0	0	0	

C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H
2	13	6	3	110	14	25	101	1	8	37
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H
0	0	9	75	3	1	7	2	7	1	1
C6H	D6	C6V	D3H	D6H	T	TH	0	TD	OH	TOTAL
0	5	0	2	0	3	0	0	10	12	458

### AB2X6

C1 -1										
0										
CI -1										
6										
C2 -1	C2 -2	C2 -3								
0	2	7								
CS -1	CS -2	CS -3	CS -4							
0	1	0	1							
C2H-1	C2H-2	C2H-3	C2H-4	C2H-5	C2H-6					
0	2	12	7	33	16					
D2 -1	D2 -2	D2 -3	D2 -4	D2 -5	D2 -6	D2 -7	D2 -8	D2 -9		
0	0	2	11	2	2	0	0	0		
C2V-1	C2V-2	C2V-3	C2V-4	C2V-5	C2V-6	C2V-7	C2V-8	C2V-9	C2V-10	
0	0	0	0	3	0	1	0	1	0	
C2V-11	C2V-12	C2V-13	C2V-14	C2V-15	C2V-16	C2V-17	C2V-18	C2V-19	C2V-20	
0	1	0	1	0	0	1	0	6	0	
C2V-21	C2V-22									
0	0									
D2H-1	D2H-2	D2H-3	D2H-4	D2H-5	D2H-6	D2H-7	D2H-8	D2H-9	D2H-10	
2	0	0	0	1	0	1	0	0	0	
D2H-11	D2H-12	D2H-13	D2H-14	D2H-15	D2H-16	D2H-17	D2H-18	D2H-19	D2H-20	
0	0	0	12	5	6	5	4	1	0	
D2H-21	D2H-22	D2H-23	D2H-24	D2H-25	D2H-26	D2H-27	D2H-28			
0	0	0	1	1	0	0	0			
C4 -1	C4 -2	C4 -3	C4 -4	C4 -5	C4 -6					
0	0	0	0	0	0					
S4 -1	S4 -2									
0	0									
C4H-1	C4H-2	C4H-3	C4H-4	C4H-5	C4H-6					
0	2	0	0	2	0					
D4 -1	D4 -2	D4 -3	D4 -4	D4 -5	D4 -6	D4 -7	D4 -8	D4 -9	D4 -10	
0	1	0	0	0	1	0	0	3	0	
C4V-1	C4V-2	C4V-3	C4V-4	C4V-5	C4V-6	C4V-7	C4V-8	C4V-9	C4V-10	
0	0	0	0	1	0	0	0	0	0	
C4V-11	C4V-12									
0	0									
D2D-1	D2D-2	D2D-3	D2D-4	D2D-5	D2D-6	D2D-7	D2D-8	D2D-9	D2D-10	
0	0	0	0	0	0	1	1	0	0	

D2D-11	D2D-12										
1	0										
D4H-1	D4H-2	D4H-3	D4H-4	D4H-5	D4H-6	D4H-7	D4H-8	D4H-9	D4H-10		
4	0	0	0	0	4	0	0	0	0		
D4H-11	D4H-12	D4H-13	D4H-14	D4H-15	D4H-16	D4H-17	D4H-18	D4H-19	D4H-20		
0	0	0	17	0	0	1	0	0	1		
C3 -1	C3 -2	C3 -3	C3 -4								
1	0	0	0								
C3I-1	C3I-2										
4	2										
D3 -1	D3 -2	D3 -3	D3 -4	D3 -5	D3 -6	D3 -7					
3	13	0	0	0	0	1					
C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6						
2	0	0	0	3	0						
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6						
7	0	25	1	3	0						
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6						
0	0	0	0	0	1						
C3H-1											
1											
C6H-1	C6H-2										
0	0										
D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6						
0	0	0	0	0	0						
C6V-1	C6V-2	C6V-3	C6V-4								
0	0	0	5								
D3H-1	D3H-2	D3H-3	D3H-4								
0	0	6	0								
D6H-1	D6H-2	D6H-3	D6H-4								
1	0	0	1								
T -1	T -2	T -3	T -4	T -5							
0	0	0	1	0							
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6	TH -7					
2	0	2	0	0	4	1					
O -1	O -2	O -3	O -4	O -5	O -6	O -7	O -8				
0	0	2	0	0	0	0	0				
TD -1	TD -2	TD -3	TD -4	TD -5	TD -6						
0	0	0	0	0	0						
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6	OH -7	OH -8	OH -9	OH -10		
0	0	0	0	68	0	67	0	0	0		
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
0	6	9	2	70	17	14	39	0	0	4	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
5	1	3	27	1	6	17	5	36	1	1	
C6H	D6	C6V	D3H	D6H	T	TH	0	TD	OH	TOTAL	
0	0	5	6	2	1	9	2	0	135	424	

## AX3

C1 -1									
0									
CI -1									
10									
C2 -1	C2 -2	C2 -3							
0	1	0							
CS -1	CS -2	CS -3	CS -4						
0	0	0	0						
C2H-1	C2H-2	C2H-3	C2H-4	C2H-5	C2H-6				
0	6	16	1	17	2				
D2 -1	D2 -2	D2 -3	D2 -4	D2 -5	D2 -6	D2 -7	D2 -8	D2 -9	
1	0	1	8	0	0	0	0	0	
C2V-1	C2V-2	C2V-3	C2V-4	C2V-5	C2V-6	C2V-7	C2V-8	C2V-9	C2V-10
0	2	0	0	0	0	1	0	4	0
C2V-11	C2V-12	C2V-13	C2V-14	C2V-15	C2V-16	C2V-17	C2V-18	C2V-19	C2V-20
0	2	0	1	0	2	1	0	0	0
C2V-21	C2V-22								
0	0								
D2H-1	D2H-2	D2H-3	D2H-4	D2H-5	D2H-6	D2H-7	D2H-8	D2H-9	D2H-10
0	0	0	0	0	0	1	0	0	0
D2H-11	D2H-12	D2H-13	D2H-14	D2H-15	D2H-16	D2H-17	D2H-18	D2H-19	D2H-20
0	0	2	0	0	20	14	0	0	1
D2H-21	D2H-22	D2H-23	D2H-24	D2H-25	D2H-26	D2H-27	D2H-28		
0	0	0	2	0	1	0	0		
C4 -1	C4 -2	C4 -3	C4 -4	C4 -5	C4 -6				
0	0	0	0	0	0				
S4 -1	S4 -2								
0	0								
C4H-1	C4H-2	C4H-3	C4H-4	C4H-5	C4H-6				
0	0	0	0	0	1				
D4 -1	D4 -2	D4 -3	D4 -4	D4 -5	D4 -6	D4 -7	D4 -8	D4 -9	D4 -10
0	0	0	0	0	0	0	0	0	0
C4V-1	C4V-2	C4V-3	C4V-4	C4V-5	C4V-6	C4V-7	C4V-8	C4V-9	C4V-10
0	0	0	0	0	0	0	0	0	0
C4V-11	C4V-12								
0	0								
D2D-1	D2D-2	D2D-3	D2D-4	D2D-5	D2D-6	D2D-7	D2D-8	D2D-9	D2D-10
0	0	1	1	0	0	0	0	0	0
D2D-11	D2D-12								
0	0								
D4H-1	D4H-2	D4H-3	D4H-4	D4H-5	D4H-6	D4H-7	D4H-8	D4H-9	D4H-10
2	0	0	0	0	0	1	0	0	0
D4H-11	D4H-12	D4H-13	D4H-14	D4H-15	D4H-16	D4H-17	D4H-18	D4H-19	D4H-20
0	0	0	0	0	0	0	6	1	0
C3 -1	C3 -2	C3 -3	C3 -4						
2	0	0	1						
C3I-1	C3I-2								

			0	11							
D3 -1	D3 -2	D3 -3	D3 -4	D3 -5	D3 -6	D3 -7					
0	5	2	0	1	0	2					
C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6						
0	0	1	0	0	0						
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6						
3	2	1	5	5	22						
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6						
0	0	0	0	0	2						
C3H-1											
0											
C6H-1	C6H-2										
0	41										
D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6						
0	1	0	0	0	5						
C6V-1	C6V-2	C6V-3	C6V-4								
0	0	3	1								
D3H-1	D3H-2	D3H-3	D3H-4								
0	1	0	0								
D6H-1	D6H-2	D6H-3	D6H-4								
1	0	7	4								
T -1	T -2	T -3	T -4	T -5							
1	0	0	0	0							
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6	TH -7					
0	0	0	0	9	0	0					
O -1	O -2	O -3	O -4	O -5	O -6	O -7	O -8	O -9	O -10		
0	0	0	0	0	0	0	0	0	0		
TD -1	TD -2	TD -3	TD -4	TD -5	TD -6						
1	0	0	0	0	0						
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6	OH -7	OH -8	OH -9	OH -10		
10	0	1	0	11	0	3	0	0	0	0	
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
0	10	1	0	42	10	13	41	0	0	1	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
0	0	2	10	3	11	10	1	38	2	0	
C6H	D6	C6V	D3H	D6H	T	TH	0	TD	OH	TOTAL	
41	6	4	1	12	1	9	0	1	25	295	

## ABX2

C1 -1											
1											
CI -1											
5											
C2 -1	C2 -2	C2 -3									
0	0	0									
CS -1	CS -2	CS -3	CS -4								

0	0	1	2							
C2H-1	C2H-2	C2H-3	C2H-4	C2H-5	C2H-6					
0	1	7	2	18	11					
D2 -1	D2 -2	D2 -3	D2 -4	D2 -5	D2 -6	D2 -7	D2 -8	D2 -9		
0	0	0	1	0	0	0	1	0		
C2V-1	C2V-2	C2V-3	C2V-4	C2V-5	C2V-6	C2V-7	C2V-8	C2V-9	C2V-10	
2	1	0	0	0	0	0	0	12	0	
C2V-11	C2V-12	C2V-13	C2V-14	C2V-15	C2V-16	C2V-17	C2V-18	C2V-19	C2V-20	
0	1	0	0	0	0	0	0	0	0	2
C2V-21	C2V-22									
0	0									
D2H-1	D2H-2	D2H-3	D2H-4	D2H-5	D2H-6	D2H-7	D2H-8	D2H-9	D2H-10	
1	0	0	0	0	0	1	1	0	0	
D2H-11	D2H-12	D2H-13	D2H-14	D2H-15	D2H-16	D2H-17	D2H-18	D2H-19	D2H-20	
2	2	2	1	4	12	11	0	0	0	
D2H-21	D2H-22	D2H-23	D2H-24	D2H-25	D2H-26	D2H-27	D2H-28			
1	0	0	0	2	1	0	1			
C4 -1	C4 -2	C4 -3	C4 -4	C4 -5	C4 -6					
0	1	0	0	0	0					
S4 -1	S4 -2									
0	2									
C4H-1	C4H-2	C4H-3	C4H-4	C4H-5	C4H-6					
1	0	0	0	1	0					
D4 -1	D4 -2	D4 -3	D4 -4	D4 -5	D4 -6	D4 -7	D4 -8	D4 -9	D4 -10	
0	0	0	1	0	0	0	0	0	0	
C4V-1	C4V-2	C4V-3	C4V-4	C4V-5	C4V-6	C4V-7	C4V-8	C4V-9	C4V-10	
0	0	0	0	0	0	0	0	0	0	1
C4V-11	C4V-12									
1	0									
D2D-1	D2D-2	D2D-3	D2D-4	D2D-5	D2D-6	D2D-7	D2D-8	D2D-9	D2D-10	
1	0	0	0	0	0	0	0	1	0	
D2D-11	D2D-12									
0	40									
D4H-1	D4H-2	D4H-3	D4H-4	D4H-5	D4H-6	D4H-7	D4H-8	D4H-9	D4H-10	
0	0	0	0	0	0	7	0	0	0	
D4H-11	D4H-12	D4H-13	D4H-14	D4H-15	D4H-16	D4H-17	D4H-18	D4H-19	D4H-20	
0	0	0	0	0	0	0	11	10	0	
C3 -1	C3 -2	C3 -3	C3 -4							
0	0	0	1							
C3I-1	C3I-2									
2	2									
D3 -1	D3 -2	D3 -3	D3 -4	D3 -5	D3 -6	D3 -7				
0	0	0	2	0	0	3				
C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6					
2	0	0	0	7	0					
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6					
1	0	4	0	81	2					
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6					
0	0	0	0	0	0					

C3H-1											
0											
C6H-1	C6H-2										
0	0										
D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6						
0	0	0	2	0	0						
C6V-1	C6V-2	C6V-3	C6V-4								
0	0	0	0								
D3H-1	D3H-2	D3H-3	D3H-4								
4	0	0	0								
D6H-1	D6H-2	D6H-3	D6H-4								
0	0	0	13								
T -1	T -2	T -3	T -4	T -5							
0	0	0	0	0							
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6	TH -7					
0	0	0	0	0	0	0					
O -1	O -2	O -3	O -4	O -5	O -6	O -7	O -8				
0	0	0	1	0	0	0	0				
TD -1	TD -2	TD -3	TD -4	TD -5	TD -6						
0	0	0	0	0	1						
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6	OH -7	OH -8	OH -9	OH -10		
3	0	0	0	2	0	5	0	1	0		
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
1	5	0	3	39	2	18	42	1	2	2	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
1	2	42	28	1	4	5	9	88	0	0	
C6H	D6	C6V	D3H	D6H	T	TH	0	TD	OH	TOTAL	
0	2	0	4	13	0	0	1	1	11	327	

### ABC2X6

C1 -1											
0											
CI -1											
3											
C2 -1	C2 -2	C2 -3									
0	1	0									
CS -1	CS -2	CS -3	CS -4								
0	0	0	0								
C2H-1	C2H-2	C2H-3	C2H-4	C2H-5	C2H-6						
0	1	4	1	15	13						
D2 -1	D2 -2	D2 -3	D2 -4	D2 -5	D2 -6	D2 -7	D2 -8	D2 -9			
0	0	0	1	0	0	0	0	0			
C2V-1	C2V-2	C2V-3	C2V-4	C2V-5	C2V-6	C2V-7	C2V-8	C2V-9	C2V-10		
1	2	0	0	0	0	0	0	0	1	1	
C2V-11	C2V-12	C2V-13	C2V-14	C2V-15	C2V-16	C2V-17	C2V-18	C2V-19	C2V-20		
0	0	0	0	0	0	0	0	1	0		

C2V-21	C2V-22										
0	0										
D2H-1	D2H-2	D2H-3	D2H-4	D2H-5	D2H-6	D2H-7	D2H-8	D2H-9	D2H-10		
0	0	0	0	0	0	0	0	1	0		
D2H-11	D2H-12	D2H-13	D2H-14	D2H-15	D2H-16	D2H-17	D2H-18	D2H-19	D2H-20		
0	0	0	0	3	2	0	0	5	0		
D2H-21	D2H-22	D2H-23	D2H-24	D2H-25	D2H-26	D2H-27	D2H-28				
0	0	0	0	3	0	0	0				
C4 -1	C4 -2	C4 -3	C4 -4	C4 -5	C4 -6						
0	0	0	0	0	0						
S4 -1	S4 -2										
1	0										
C4H-1	C4H-2	C4H-3	C4H-4	C4H-5	C4H-6						
0	0	0	0	3	2						
D4 -1	D4 -2	D4 -3	D4 -4	D4 -5	D4 -6	D4 -7	D4 -8	D4 -9	D4 -10		
0	0	0	0	0	0	0	0	0	0		
C4V-1	C4V-2	C4V-3	C4V-4	C4V-5	C4V-6	C4V-7	C4V-8	C4V-9	C4V-10		
0	0	0	0	0	0	0	0	0	0		
C4V-11	C4V-12										
0	0										
D2D-1	D2D-2	D2D-3	D2D-4	D2D-5	D2D-6	D2D-7	D2D-8	D2D-9	D2D-10		
0	0	0	0	0	0	0	0	0	0		
D2D-11	D2D-12										
0	0										
D4H-1	D4H-2	D4H-3	D4H-4	D4H-5	D4H-6	D4H-7	D4H-8	D4H-9	D4H-10		
0	0	1	0	0	0	0	0	0	0		
D4H-11	D4H-12	D4H-13	D4H-14	D4H-15	D4H-16	D4H-17	D4H-18	D4H-19	D4H-20		
0	0	0	0	0	0	5	0	0	2		
C3 -1	C3 -2	C3 -3	C3 -4								
0	0	0	0								
C3I-1	C3I-2										
0	6										
D3 -1	D3 -2	D3 -3	D3 -4	D3 -5	D3 -6	D3 -7					
0	1	0	0	0	0	1					
C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6						
2	0	0	0	0	0						
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6						
0	0	3	0	6	0						
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6						
0	0	0	0	0	0						
C3H-1											
0											
C6H-1	C6H-2										
0	0										
D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6						
0	0	0	0	0	0						
C6V-1	C6V-2	C6V-3	C6V-4								
0	0	0	1								
D3H-1	D3H-2	D3H-3	D3H-4								

0	0	0	0								
D6H-1	D6H-2	D6H-3	D6H-4								
0	0	0	2								
T -1	T -2	T -3	T -4	T -5							
0	0	0	0	0							
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6	TH -7					
0	0	2	0	0	4	0					
O -1	O -2	O -3	O -4	O -5	O -6	O -7	O -8				
0	0	0	0	0	0	0	0				
TD -1	TD -2	TD -3	TD -4	TD -5	TD -6						
0	0	0	0	0	0						
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6	OH -7	OH -8	OH -9	OH -10		
0	0	0	0	36	0	0	0	0	0		
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
0	3	1	0	34	1	6	14	0	1	5	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
0	0	0	8	0	6	2	2	9	0	0	
C6H	D6	C6V	D3H	D6H	T	TH	0	TD	OH	TOTAL	
0	0	1	0	2	0	6	0	0	36	137	

N02

C1 -1											
1											
CI -1											
0											
C2 -1	C2 -2	C2 -3									
0	1	4									
CS -1	CS -2	CS -3	CS -4								
0	1	1	0								
C2H-1	C2H-2	C2H-3	C2H-4	C2H-5	C2H-6						
0	3	8	2	4	1						
D2 -1	D2 -2	D2 -3	D2 -4	D2 -5	D2 -6	D2 -7	D2 -8	D2 -9			
1	0	0	0	0	1	0	0	0			
C2V-1	C2V-2	C2V-3	C2V-4	C2V-5	C2V-6	C2V-7	C2V-8	C2V-9	C2V-10		
0	0	0	1	0	0	1	0	1	1		
C2V-11	C2V-12	C2V-13	C2V-14	C2V-15	C2V-16	C2V-17	C2V-18	C2V-19	C2V-20		
0	1	0	0	0	0	0	0	0	0		
C2V-21	C2V-22										
0	1										
D2H-1	D2H-2	D2H-3	D2H-4	D2H-5	D2H-6	D2H-7	D2H-8	D2H-9	D2H-10		
0	0	0	0	1	0	0	0	2	0		
D2H-11	D2H-12	D2H-13	D2H-14	D2H-15	D2H-16	D2H-17	D2H-18	D2H-19	D2H-20		
1	18	1	1	1	11	6	1	0	0		
D2H-21	D2H-22	D2H-23	D2H-24	D2H-25	D2H-26	D2H-27	D2H-28				
0	0	0	3	2	0	0	0				
C4 -1	C4 -2	C4 -3	C4 -4	C4 -5	C4 -6						

0	0	0	0	2	0						
S4 -1	S4 -2										
0	0										
C4H-1	C4H-2	C4H-3	C4H-4	C4H-5	C4H-6						
0	0	0	0	3	0						
D4 -1	D4 -2	D4 -3	D4 -4	D4 -5	D4 -6	D4 -7	D4 -8	D4 -9	D4 -10		
0	0	0	1	0	0	0	1	0	1		
C4V-1	C4V-2	C4V-3	C4V-4	C4V-5	C4V-6	C4V-7	C4V-8	C4V-9	C4V-10		
1	0	0	1	0	0	0	0	1	0		
C4V-11	C4V-12										
0	0										
D2D-1	D2D-2	D2D-3	D2D-4	D2D-5	D2D-6	D2D-7	D2D-8	D2D-9	D2D-10		
0	0	0	0	0	0	0	0	0	0		
D2D-11	D2D-12										
3	0										
D4H-1	D4H-2	D4H-3	D4H-4	D4H-5	D4H-6	D4H-7	D4H-8	D4H-9	D4H-10		
1	0	0	0	0	0	0	12	0	0		
D4H-11	D4H-12	D4H-13	D4H-14	D4H-15	D4H-16	D4H-17	D4H-18	D4H-19	D4H-20		
0	0	0	0	0	0	20	5	19	1		
C3 -1	C3 -2	C3 -3	C3 -4								
1	0	0	0								
C3I-1	C3I-2										
1	1										
D3 -1	D3 -2	D3 -3	D3 -4	D3 -5	D3 -6	D3 -7					
1	0	0	0	0	0	0					
C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6						
1	0	0	1	1	0						
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6						
2	0	7	0	7	0						
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6						
0	0	0	0	0	0						
C3H-1											
2											
C6H-1	C6H-2										
0	0										
D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6						
1	0	0	5	1	0						
C6V-1	C6V-2	C6V-3	C6V-4								
0	0	0	0								
D3H-1	D3H-2	D3H-3	D3H-4								
1	0	3	1								
D6H-1	D6H-2	D6H-3	D6H-4								
44	0	0	20								
T -1	T -2	T -3	T -4	T -5							
0	0	0	0	1							
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6	TH -7					
0	1	0	0	0	7	1					
O -1	O -2	O -3	O -4	O -5	O -6	O -7	O -8				
0	0	0	0	0	2	1	0				

TD -1	TD -2	TD -3	TD -4	TD -5	TD -6						
0	0	1	0	0	0						
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6	OH -7	OH -8	OH -9	OH -10		
0	0	0	0	8	0	4	0	0	0		
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
1	0	5	2	18	2	6	48	2	0	3	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
3	3	3	58	1	2	1	3	16	0	2	
C6H	D6	C6V	D3H	D6H	T	TH	0	TD	OH	TOTAL	
0	7	0	5	64	1	9	3	1	12	281	

## A2X3

C1 -1											
1											
CI -1											
0											
C2 -1	C2 -2	C2 -3									
0	1	0									
CS -1	CS -2	CS -3	CS -4								
0	0	1	4								
C2H-1	C2H-2	C2H-3	C2H-4	C2H-5	C2H-6						
0	6	8	0	6	1						
D2 -1	D2 -2	D2 -3	D2 -4	D2 -5	D2 -6	D2 -7	D2 -8	D2 -9			
0	0	0	0	0	0	0	0	0			
C2V-1	C2V-2	C2V-3	C2V-4	C2V-5	C2V-6	C2V-7	C2V-8	C2V-9	C2V-10		
0	0	0	0	0	0	0	0	0	0		
C2V-11	C2V-12	C2V-13	C2V-14	C2V-15	C2V-16	C2V-17	C2V-18	C2V-19	C2V-20		
0	3	0	0	0	0	0	0	0	2	0	
C2V-21	C2V-22										
0	0										
D2H-1	D2H-2	D2H-3	D2H-4	D2H-5	D2H-6	D2H-7	D2H-8	D2H-9	D2H-10		
0	0	0	0	0	0	0	0	1	1		
D2H-11	D2H-12	D2H-13	D2H-14	D2H-15	D2H-16	D2H-17	D2H-18	D2H-19	D2H-20		
0	0	0	2	2	10	0	0	0	0		
D2H-21	D2H-22	D2H-23	D2H-24	D2H-25	D2H-26	D2H-27	D2H-28				
0	0	0	1	0	0	0	0				
C4 -1	C4 -2	C4 -3	C4 -4	C4 -5	C4 -6						
0	0	0	0	0	0						
S4 -1	S4 -2										
0	0										
C4H-1	C4H-2	C4H-3	C4H-4	C4H-5	C4H-6						
0	0	0	0	0	0						
D4 -1	D4 -2	D4 -3	D4 -4	D4 -5	D4 -6	D4 -7	D4 -8	D4 -9	D4 -10		
0	0	0	0	0	0	0	0	0	0		
C4V-1	C4V-2	C4V-3	C4V-4	C4V-5	C4V-6	C4V-7	C4V-8	C4V-9	C4V-10		
0	0	0	0	0	0	0	0	0	0		

C4V-11	C4V-12										
0	0										
D2D-1	D2D-2	D2D-3	D2D-4	D2D-5	D2D-6	D2D-7	D2D-8	D2D-9	D2D-10		
0	0	0	0	0	0	2	0	0	0		
D2D-11	D2D-12										
0	0										
D4H-1	D4H-2	D4H-3	D4H-4	D4H-5	D4H-6	D4H-7	D4H-8	D4H-9	D4H-10		
1	0	0	0	0	0	0	0	0	0		
D4H-11	D4H-12	D4H-13	D4H-14	D4H-15	D4H-16	D4H-17	D4H-18	D4H-19	D4H-20		
0	0	0	0	0	0	0	0	1	1		
C3 -1	C3 -2	C3 -3	C3 -4								
1	1	0	0								
C3I-1	C3I-2										
0	2										
D3 -1	D3 -2	D3 -3	D3 -4	D3 -5	D3 -6	D3 -7					
0	4	0	0	0	0	2					
C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6						
0	0	0	0	2	0						
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6						
0	2	6	0	5	12						
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6						
0	0	0	0	0	0						
C3H-1											
0											
C6H-1	C6H-2										
0	0										
D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6						
0	0	0	0	0	0						
C6V-1	C6V-2	C6V-3	C6V-4								
0	0	0	1								
D3H-1	D3H-2	D3H-3	D3H-4								
0	0	0	0								
D6H-1	D6H-2	D6H-3	D6H-4								
0	0	0	4								
T -1	T -2	T -3	T -4	T -5							
0	0	1	0	15							
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6	TH -7					
0	0	0	0	0	0	14					
O -1	O -2	O -3	O -4	O -5	O -6	O -7	O -8				
0	0	0	0	0	0	0	0				
TD -1	TD -2	TD -3	TD -4	TD -5	TD -6						
0	0	0	0	0	4						
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6	OH -7	OH -8	OH -9	OH -10		
0	0	0	2	2	0	2	0	1	0		
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H	
1	0	1	5	21	0	5	17	0	0	0	
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H	
0	0	2	3	2	2	6	2	25	0	0	

C6H	D6	C6V	D3H	D6H	T	TH	O	TD	OH	TOTAL
0	0	1	0	4	16	14	0	4	7	138

NO

C1 -1										
	0									
CI -1										
	0									
C2 -1	C2 -2	C2 -3								
	0	0	0							
CS -1	CS -2	CS -3	CS -4							
	0	0	0	1						
C2H-1	C2H-2	C2H-3	C2H-4	C2H-5	C2H-6					
	0	0	3	1	5	3				
D2 -1	D2 -2	D2 -3	D2 -4	D2 -5	D2 -6	D2 -7	D2 -8	D2 -9		
	0	0	0	2	1	0	0	0	0	
C2V-1	C2V-2	C2V-3	C2V-4	C2V-5	C2V-6	C2V-7	C2V-8	C2V-9	C2V-10	
	1	0	0	0	0	0	0	0	0	
C2V-11	C2V-12	C2V-13	C2V-14	C2V-15	C2V-16	C2V-17	C2V-18	C2V-19	C2V-20	
	0	1	0	0	0	0	0	0	0	
C2V-21	C2V-22									
	0	0								
D2H-1	D2H-2	D2H-3	D2H-4	D2H-5	D2H-6	D2H-7	D2H-8	D2H-9	D2H-10	
	1	0	0	0	0	0	1	0	0	
D2H-11	D2H-12	D2H-13	D2H-14	D2H-15	D2H-16	D2H-17	D2H-18	D2H-19	D2H-20	
	0	0	1	1	3	34	6	0	0	
D2H-21	D2H-22	D2H-23	D2H-24	D2H-25	D2H-26	D2H-27	D2H-28			
	0	0	0	0	0	0	0			
C4 -1	C4 -2	C4 -3	C4 -4	C4 -5	C4 -6					
	1	0	0	0	0					
S4 -1	S4 -2									
	0	0								
C4H-1	C4H-2	C4H-3	C4H-4	C4H-5	C4H-6					
	0	0	0	0	0					
D4 -1	D4 -2	D4 -3	D4 -4	D4 -5	D4 -6	D4 -7	D4 -8	D4 -9	D4 -10	
	0	0	0	0	0	0	0	0	0	
C4V-1	C4V-2	C4V-3	C4V-4	C4V-5	C4V-6	C4V-7	C4V-8	C4V-9	C4V-10	
	0	0	0	0	0	0	0	3	0	
C4V-11	C4V-12									
	0	0								
D2D-1	D2D-2	D2D-3	D2D-4	D2D-5	D2D-6	D2D-7	D2D-8	D2D-9	D2D-10	
	0	0	0	0	0	0	0	0	0	
D2D-11	D2D-12									
	0	0								
D4H-1	D4H-2	D4H-3	D4H-4	D4H-5	D4H-6	D4H-7	D4H-8	D4H-9	D4H-10	
	0	0	0	0	1	0	1	0	0	
D4H-11	D4H-12	D4H-13	D4H-14	D4H-15	D4H-16	D4H-17	D4H-18	D4H-19	D4H-20	

0	0	0	0	0	0	0	2	1	4	1
C3 -1	C3 -2	C3 -3	C3 -4							
0	1	0	0							
C3I-1	C3I-2									
0	0									
D3 -1	D3 -2	D3 -3	D3 -4	D3 -5	D3 -6	D3 -7				
0	0	0	1	0	0	0				
C3V-1	C3V-2	C3V-3	C3V-4	C3V-5	C3V-6					
0	0	0	0	4	0					
D3D-1	D3D-2	D3D-3	D3D-4	D3D-5	D3D-6					
1	0	3	0	3	0					
C6 -1	C6 -2	C6 -3	C6 -4	C6 -5	C6 -6					
0	0	0	0	0	0					
C3H-1										
0										
C6H-1	C6H-2									
0	0									
D6 -1	D6 -2	D6 -3	D6 -4	D6 -5	D6 -6					
0	0	0	0	0	1					
C6V-1	C6V-2	C6V-3	C6V-4							
0	0	0	4							
D3H-1	D3H-2	D3H-3	D3H-4							
1	0	4	0							
D6H-1	D6H-2	D6H-3	D6H-4							
1	0	0	20							
T -1	T -2	T -3	T -4	T -5						
1	1	0	8	0						
TH -1	TH -2	TH -3	TH -4	TH -5	TH -6	TH -7				
0	0	0	0	0	0	0				
O -1	O -2	O -3	O -4	O -5	O -6	O -7	O -8	O -9	O -10	
0	0	0	0	0	0	0	0	0	0	
TD -1	TD -2	TD -3	TD -4	TD -5	TD -6					
0	2	0	0	0	0					
OH -1	OH -2	OH -3	OH -4	OH -5	OH -6	OH -7	OH -8	OH -9	OH -10	
2	0	1	1	33	0	2	0	0	0	
C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H
0	0	0	1	12	3	2	47	1	0	0
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H
0	3	0	10	1	0	1	4	7	0	0
C6H	D6	C6V	D3H	D6H	T	TH	0	TD	OH	TOTAL
0	1	4	5	21	10	0	0	2	39	174

*DIFF2 : 0.025*

C1	CI	C2	CS	C2H	D2	C2V	D2H	C4	S4	C4H
D4	C4V	D2D	D4H	C3	C3I	D3	C3V	D3D	C6	C3H
C6H	D6	C6V	D3H	D6H	T	TH	O	TD	OH	TOTAL
<b>ABX3(DIFF2:0.025)</b>										
3	16	5	10	72	11	23	186	1	1	5
0	12	3	16	7	22	2	32	44	4	0
2	4	17	5	64	7	2	1	3	117	697
<b>AB2X4(DIFF2:0.025)</b>										
2	9	8	5	55	1	26	167	1	22	7
2	1	13	68	0	8	1	2	15	3	0
2	3	2	1	6	1	4	0	4	102	541
<b>AX2(DIFF2:0.025)</b>										
3	4	3	4	54	13	21	84	1	1	9
18	0	7	78	0	2	14	22	53	0	1
1	3	5	3	13	2	31	1	4	85	540
<b>AX(DIFF2:0.025)</b>										
0	3	2	0	33	4	16	55	2	4	3
0	1	3	32	0	0	4	11	23	2	3
0	0	24	6	17	35	0	0	28	184	495
<b>ABX4(DIFF2:0.025)</b>										
2	15	7	3	113	15	26	104	1	8	40
0	0	10	76	3	1	7	2	7	1	1
0	5	0	2	0	3	0	0	10	12	474
<b>AB2X6(DIFF2:0.025)</b>										
0	6	9	2	72	18	15	40	0	0	4
5	1	3	27	1	7	17	5	36	1	1
0	0	5	6	2	1	9	2	0	141	436
<b>AX3(DIFF2:0.025)</b>										
0	10	1	0	42	10	13	41	0	0	1
0	0	2	10	3	11	10	1	38	2	0
42	6	4	1	12	1	9	0	1	25	296
<b>ABX2(DIFF2:0.025)</b>										
1	5	0	3	39	2	18	42	1	2	2
1	2	43	28	1	4	5	9	89	0	0
0	2	0	4	13	0	0	1	1	11	329
<b>ABC2X6(DIFF2:0.025)</b>										
0	3	1	0	39	2	6	14	0	1	5
0	0	0	9	0	7	2	2	9	0	0
0	0	1	0	2	0	6	0	0	46	155
<b>N02(DIFF2:0.025)</b>										
1	0	5	2	18	2	6	48	2	0	3
3	3	3	59	1	2	1	3	16	0	2
0	7	0	5	65	1	10	3	1	12	284
<b>A2X3(DIFF2:0.025)</b>										
1	0	1	5	22	0	5	17	0	0	0
0	0	2	3	2	2	6	2	27	0	0
0	0	1	0	4	16	15	0	4	8	143
<b>NO(DIFF2:0.025)</b>										

0	0	0	1	12	3	2	51	1	0	0
0	3	0	10	1	0	1	4	7	0	0
0	1	4	5	22	10	0	0	2	39	179
<b>AXY(DIFF2:0.025)</b>										
0	1	0	0	18	2	5	50	0	0	2
0	0	2	72	1	2	0	1	12	0	1
0	0	2	0	3	4	0	0	1	2	181
<b>AB2X5(DIFF2:0.025)</b>										
2	7	3	1	40	3	11	44	0	0	0
0	1	1	8	0	0	1	0	0	2	0
0	0	0	0	1	0	0	1	0	0	126
<b>A3X4(DIFF2:0.025)</b>										
0	0	0	0	5	0	5	2	0	0	0
1	0	2	2	0	2	0	2	2	1	0
4	0	0	0	1	0	0	0	17	45	91
<b>N(DIFF2:0.025)</b>										
0	0	3	0	21	1	2	16	2	0	2
1	1	1	5	1	2	6	0	11	0	0
0	0	2	1	16	4	5	0	1	15	119
<b>A2B2X7(DIFF2:0.025)</b>										
2	23	5	0	40	1	12	6	5	0	0
2	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	1	41	138
<b>ABX6(DIFF2:0.025)</b>										
0	2	3	4	18	2	1	11	0	1	2
0	0	5	3	1	38	0	0	18	0	0
0	0	0	0	0	0	9	0	0	9	127
<b>AB2X2(DIFF2:0.025)</b>										
0	3	0	0	9	2	1	26	0	0	0
4	3	1	52	0	2	0	1	39	0	0
0	3	0	0	1	0	0	0	2	0	149
<b>NOP(DIFF2:0.025)</b>										
1	1	1	0	8	0	7	24	0	0	1
1	3	1	37	2	0	0	0	6	0	0
0	0	4	17	21	3	0	0	4	0	142
<b>ABCX4(DIFF2:0.025)</b>										
0	4	2	2	11	2	17	28	0	0	1
0	0	0	0	2	0	0	3	1	6	0
0	5	1	0	2	1	0	0	1	0	89
<b>AB3X6(DIFF2:0.025)</b>										
0	4	4	0	26	2	7	14	0	0	1
1	0	0	4	1	6	3	0	4	0	0
1	1	0	0	0	0	4	0	3	16	102
<b>AB2X3(DIFF2:0.025)</b>										
0	4	0	2	35	2	13	44	0	0	0
1	0	0	2	1	1	2	1	3	0	0
0	1	0	0	5	0	0	0	0	0	117
<b>NO2P2(DIFF2:0.025)</b>										
0	0	0	0	3	2	0	15	0	0	0

0	0	1	82	0	1	0	0	18	0	0	0
0	2	0	0	5	0	1	0	0	0	0	130
<b>A2B3C3X12(0.025)</b>											
0	1	0	0	8	0	1	2	0	0	0	1
0	0	1	0	0	1	0	2	1	0	0	0
0	0	0	1	0	0	0	0	0	25	44	
<b>ABX5(DIFF2:0.025)</b>											
0	8	5	2	20	5	3	12	2	0	5	
0	0	0	0	0	3	1	1	2	1	0	
0	0	0	0	1	0	0	0	0	1	72	
<b>A2B3X8(DIFF2:0.025)</b>											
0	2	2	1	36	0	1	11	0	0	0	
0	0	2	0	0	0	0	5	11	0	0	
1	0	6	1	0	1	0	1	1	1	83	
<b>AX4(DIFF2:0.025)</b>											
0	4	1	1	29	3	4	13	1	0	4	
0	1	1	13	0	0	0	1	1	0	0	
0	0	0	0	0	1	4	1	2	3	88	
<b>AB2X8(DIFF2:0.025)</b>											
0	10	1	1	31	7	4	17	0	0	0	
1	1	0	1	1	3	0	1	3	0	1	
0	0	0	1	1	0	0	0	0	0	85	
<b>AB4X8(DIFF2:0.025)</b>											
1	7	0	0	12	0	1	5	0	0	6	
0	0	0	0	0	0	0	0	1	0	0	
0	0	0	0	2	0	0	0	2	2	39	
<b>AB2X7(DIFF2:0.025)</b>											
0	4	2	1	33	1	4	11	1	0	2	
1	0	1	2	0	0	0	0	0	0	0	
0	0	0	0	0	0	4	0	0	3	70	
<b>N03(DIFF2:0.025)</b>											
0	2	0	1	4	0	2	10	0	3	5	
0	0	3	2	0	0	2	1	12	1	0	
1	0	0	0	11	0	11	0	0	16	87	
<b>ABX(DIFF2:0.025)</b>											
0	0	0	4	1	0	2	14	0	5	0	
0	0	8	21	0	0	0	0	0	0	0	
0	0	0	4	12	1	1	0	1	4	78	
<b>AXY2(DIFF2:0.025)</b>											
1	3	2	0	12	1	5	20	0	0	5	
1	1	2	1	1	1	0	1	3	0	0	
0	0	0	0	1	0	0	0	0	0	61	
<b>TOTAL=</b>											
20	161	76	55	991	117	285	1244	21	48	116	
43	34	121	723	30	128	85	115	512	24	10	
54	43	78	63	303	92	125	11	94	965	6787	

## 5 Program lists

### 5.1 ITOH4XC.SGRL.FORT(CHARCNV3)

```
***** 00000100
*
*      TRANSFORM EBCDIC LOWERCASE LETTERS TO EBCDIK UPPERCASE LETTERS * 00000200
*                                         VER. 4.1 94.04.21      * 00000300
*                                         ***** 00000400
***** 00000500
    CHARACTER*80 ICSD          00000600
    CHARACTER*10 WSGR         00000700
    CHARACTER*1 UPPER(26),LOWER(26),V 00000800
    DATA(UPPER(I),I=1,26) /'A','B','C','D','E','F','G','H','I','J',
    -                           'K','L','M','N','O','P','Q','R','S','T',
    -                           'U','V','W','X','Y','Z'/ 00000900
    -                                         ***** 00001000
    -                                         'U','V','W','X','Y','Z'/ 00001100
    DATA(LOWER(I),I=1,26) /'a','b','c','d','e','f','g','h','i','j',
    -                           'k','l','m','n','o','p','q','r','s','t',
    -                           'u','v','w','x','y','z'/ 00001200
    -                                         ***** 00001300
    -                                         'u','v','w','x','y','z'/ 00001400
*
* 10 READ(10,6001,END=50) ICSD          00001500
6001 FORMAT(A80)          00001600
    DO 30 I=1,72          00001700
    DO 20 J=1,26          00001800
    IF(ICSD(I+8:I+8).EQ.LOWER(J)) THEN 00001900
        ICSD(I+8:I+8)=UPPER(J) 00002000
        GOTO 30          00002100
    ENDIF          00002200
20 CONTINUE          00002300
30 CONTINUE          00002400
    IF(ICSD(2:3).EQ.' 9') THEN 00002500
        WSGR=ICSD(9:18) 00002600
        CALL HSCONV(WSGR,V) 00002700
        ICSD(21:30)=WSGR 00002800
        ICSD(32:32)=V 00002900
    ENDIF          00003000
40 WRITE(11,6001) ICSD          00003100
    GOTO 10          00003200
50 STOP          00003300
    END          00003400
***** 00003500
*
*      TRANSFORM HERMANN-MAUGUIN SYMBOL TO SCHOENFLIES SYMBOL * 00003600
*                                         ***** 00003700
***** 00003800
    SUBROUTINE HSCONV(SGR,V) 00003900
    CHARACTER*10 SGR          00004000
    CHARACTER*1 V          00004100
    CHARACTER*8 HERMAN(600),HAB(55),HC(41),HF(43),HI(76),HPM1(46) 00004200
    CHARACTER*8 HPM2(86),HP12(78),HP34(60),HP46(74),HR(28) 00004300
    DIMENSION IS1(55),IS2(41),IS3(43),IS4(76),IS5(46) 00004400
    DIMENSION IS6(86),IS7(78),IS8(60),IS9(74),IS10(28) 00004500
    EQUIVALENCE (HAB(1),HERMAN(1)),(HC(1),HERMAN(56)), 00004600
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-          (HF(1),HERMAN(97)),(HI(1),HERMAN(140)),           00004700
-          (HPM1(1),HERMAN(216)),(HPM2(1),HERMAN(262)),       00004800
-          (HP12(1),HERMAN(348)),(HP34(1),HERMAN(426)),       00004900
-          (HP46(1),HERMAN(486)),(HR(1),HERMAN(560))        00005000
DATA (HAB(I),I=1,55)    /'ABA2      ','ABMA      ','ABMM      ',, 00005100
-          'ABM2      ','ACAM      ','ACMM      ','AMAM      ','AMA2      ',, 00005200
-          'AMMA      ','AMM2      ','A1-       ','A1A1      ','A11A      ',, 00005300
-          'A11M      ','A112/A   ','A112/M   ','A12/A1    ','A12/A1S   ',, 00005400
-          'A12/M1    ','A121     ','A2MM      ','A21AM    ','A21MA    ',, 00005500
-          'A2122    ','A222     ','A2/AB    ','A2/AC    ','BBA2      ',, 00005600
-          'BBCM      ','BBMM      ','BB21M    ','BMAB      ','BMABS    ',, 00005700
-          'BMAM      ','BMMB      ','BMMBS    ','BMMM      ','BMM2      ',, 00005800
-          'B1-       ','B11B     ','B11M      ','B112      ','B112/B    ',, 00005900
-          'B112/BS  ','B112/M   ','B2       ','B2/M      ','B2CB      ',, 00006000
-          'B2MB      ','B2MM      ','B2212    ','BB       ','BM       ',, 00006100
-          'B2/B      ','AA       '/,,                   00006200
DATA (HC(I),I=1,41)    /'CC       ','CCCAZ    ','CCCM      ',, 00006300
-          'CCC2      ','CCMB      ','CCMBS    ','CCMM      ','CCM21    ',, 00006400
-          'CC2A      ','CC2M      ','CM       ','CMCA      ','CMCM    ',, 00006500
-          'CMC21    ','CMMA      ','CMMM      ','CMM2      ','CM2A    ',, 00006600
-          'CM2M      ','C1       ','C1-       ','C1C1      ','C1M1    ',, 00006700
-          'C12/C1   ','C12/C1S  ','C12/M1   ','C121     ','C2       ',, 00006800
-          'C2/C      ','C2/M      ','C2CB      ','C2CM      ','C2MM    ',, 00006900
-          'C222      ','C2221    ','C2221S  ','C4-M21   ','C4-2B    ',, 00007000
-          'C4/MCC   ','C4221    ','CCCAS    '/,,                   00007100
DATA (HF(I),I=1,43)    /'FDDDS   ','FDDDZ    ','FDD2      ',, 00007200
-          'FDD2S    ','FD2D      ','FD3-CZ   ','FD3-MS   ','FD3-MS1  ',, 00007300
-          'FD3-MZ   ','FD3-S    ','FD3-Z    ','FD3MS    ','FD3MZ   ',, 00007400
-          'FD3S     ','FMMM      ','FMM2      ','FM2M      ','FM3     ',, 00007500
-          'FM3-     ','FM3-C    ','FM3-M    ','FM3C      ','FM3M    ',, 00007600
-          'F1       ','F1-      ','F2DD      ','F222     ','F23     ',, 00007700
-          'F4-D2   ','F4-3C    ','F4-3M    ','F4/MMM   ','F41/DDM  ',, 00007800
-          'F4132   ','F432     ','FD3-C    ','FD3-CS   ','FD3-M   ',, 00007900
-          'FD3-     ','FD3CS    ','FD3CZ   ','FD3C     ','FD3M   ',/,, 00008000
DATA (HI(I),I=1,76)    /'IA3      ','IA3-     ','IA3-D    ',, 00008100
-          'IA3D     ','IBAM      ','IBAMS    ','IBA2      ','IBCA    ',, 00008200
-          'IBMM     ','IBM2      ','ICMA     ','ICMAS   ','ICMM    ',, 00008300
-          'IMAM     ','IMA2      ','IMCM     ','IMMA    ','IMMM    ',, 00008400
-          'IMM2     ','IM2M      ','IM3-     ','IM3-M   ','IM3M    ',, 00008500
-          'I1       ','I1-      ','I12/C1  ','I2CM     ','I2MB    ',, 00008600
-          'I212121 ','I213     ','I222     ','I23      ','I4      ',, 00008700
-          'I4-      ','I4-C2   ','I4-M2   ','I4-2D   ','I4-2DS  ',, 00008800
-          'I4-2M   ','I4-3D   ','I4-3M   ','I4/M    ','I4/MCM  ',, 00008900
-          'I4/MCMS ','I4/MMM  ','I4CM    ','I4MM    ','I41     ',, 00009000
-          'I41/ACDS','I41/ACDZ ','I41/AMDS ','I41/AMDZ ','I41/AMD1 ',, 00009100
-          'I41/AS   ','I41/AZ   ','I41/AZ1  ','I41CD   ','I41MD   ',, 00009200
-          'I4122   ','I4132   ','I422     ','I432     ','IM3     ',, 00009300
-          'I2/C    ','I41/A    ','I41/ACD ','I41/AMD ','I4132S ',, 00009400
-          'I2/M    ',,,                   00009500

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-   'I112/B  ','I11B    ','I121    ','I12/A1  ','I12/M1  ', 00009600
-   'I1A1    ','I1M1    '/          ,          ,          ,          , 00009700
  DATA (HPM1(I),I=1,46)  //PA3      ','PA3-    ','PBAM    ', 00009800
-   'PBANS   ','PBANZ   ','PBA2    ','PBCA    ','PBCB    ', 00009900
-   'PBCM    ','PBCN    ','PBC21   ','PBC21S  ','PBMA    ', 00010000
-   'PBMM    ','PBMN    ','PBMNS   ','PBM2    ','PBNA    ', 00010100
-   'PBNB    ','PBNM    ','PBNMS   ','PBNN    ','PBN21   ', 00010200
-   'PB2N    ','PB21A   ','PB21M   ','PC      ','PCAB    ', 00010300
-   'PCAM    ','PCAN    ','PCA21   ','PCA21S  ','PCCA    ', 00010400
-   'PCCM    ','PCCN    ','PCMA    ','PCMB    ','PCMN    ', 00010500
-   'PCNB    ','PCNBS   ','PCNM    ','PCN2    ','PC21B   ', 00010600
-   'PC21N   ','PB      ','PCC2    '/          ,          , 00010700
  DATA (HPM2(I),I=1,86)  //PMAB   ','PMAM    ','PMAN    ', 00010800
-   'PMA2    ','PMCA    ','PMCB    ','PMCM    ','PMCN    ', 00010900
-   'PMCNS   ','PMCNS1  ','PMCNS2  ','PMC21   ','PMMA    ', 00011000
-   'PMMB    ','PMMM    ','PMMNS   ','PMMNZ   ',          , 00011100
-   'PMM2    ','PMNA    ','PMNB    ','PMNBS   ','PMNBS1  ', 00011200
-   'PMNM    ','PMNMS   ','PMNMZ   ','PMNN    ','PMN21   ', 00011300
-   'PMN21S  ','PM2A    ','PM2M    ','PM21B   ','PM21N   ', 00011400
-   'PM21NS  ','PM3-    ','PM3-M   ','PM3-N   ','PM3M    ', 00011500
-   'PM3N    ','PNAA    ','PNAB    ','PNAM    ','PNAMS   ', 00011600
-   'PNAN    ','PNANS   ','PNA21   ','PNCA    ','PNCM    ', 00011700
-   'PNCN    ','PNC2    ','PNMA    ','PNMM    ','PNMMS   ', 00011800
-   'PNMMZ   ','PNMN    ','PNM21   ','PNNA    ','PNNM    ', 00011900
-   'PNNNZ   ','PNN2    ','PN2B    ','PN2N    ','PN21A   ', 00012000
-   'PN21M   ','PN21MS  ','PN3-MS  ','PN3-MZ  ','PN3-NZ   ', 00012100
-   'PN3-S   ','PN3-Z   ','PM      ','PMB     ','PMC     ', 00012200
-   'PMMN    ','PM3     ','PNNNS   ','PNNN    ','PN3-M   ', 00012300
-   'PN3-N   ','PN3-    ','PN3MS   ','PN3MZ   ','PN3M    ', 00012400
-   'PN3NS   ','PN3NZ   ','PN3N    ','PN      '/          , 00012500
  DATA (HP12(I),I=1,78)  //P1     ','P1-    ','P1A1   ', 00012600
-   'P1C1    ','P1M1    ','P11A    ','P11B    ','P11M    ', 00012700
-   'P112    ','P112/A  ','P112/B  ','P112/M  ','P112/MS ', 00012800
-   'P1121   ','P1121/A ','P1121/B ','P1121/M ','P1121/N ', 00012900
-   'P12/A1  ','P12/C1  ','P12/C1S ','P12/M1  ','P121    ', 00013000
-   'P121/A1 ','P121/A1S','P121/C1 ','P121/C1S','P121/M1 ', 00013100
-   'P121/M1S','P121/N1 ','P1211   ','P2/C    ','P2CM    ', 00013200
-   'P2MM    ','P2MMS   ','P2NN    ','P21/A   ','P21/B   ', 00013300
-   'P21/C   ','P21/MB  ','P21/NB  ','P21AB   ','P21AM   ', 00013400
-   'P21CA   ','P21CN   ','P21CNS  ','P21MA   ','P21MN   ', 00013500
-   'P21MNS  ','P21NB   ','P21NM   ','P21212  ','P212121 ', 00013600
-   'P212121S','P21221  ','P213    ','P2212   ','P22121  ', 00013700
-   'P222    ','P2221   ','P23     ','P2      ','P2/B    ', 00013800
-   'P2/MB   ','P2/MC   ','P2/M    ','P2B     ','P2C     ', 00013900
-   'P21     ','P21/M   ','P21/MC  ','P21/NC  ','P21B    ', 00014000
-   'P21C   ',          ,          ,          ,          , 00014100
-   'P112/N  ','P11N    ','P12/N1  ','P1N1    '/          , 00014200
  DATA (HP34(I),I=1,60)  //P3     ','P3-    ','P3-C1  ', 00014300
-   'P3-M1   ','P3-1C  ','P3-1CS  ','P3-1M  ','P3C1    ', 00014400

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-   'P3M1    ,,'P31      ,,'P31C     ,,'P31M     ,,'P3112    ,,
-   'P3112S  ,,'P312      ,,'P3121    ,,'P3121S   ,,'P32      ,,
-   'P321    ,,'P3212    ,,'P3221    ,,'P3221S   ,,'P4       ,
-   'P4-     ,,'P4-B2     ,,'P4-B2S   ,,'P4-C2    ,,'P4-M2    ,
-   'P4-N2   ,,'P4-2C     ,,'P4-2M    ,,'P4-21C   ,,'P4-21M   ,
-   'P4-3M   ,,'P4-3N     ,,'P4/M     ,,'P4/MBM   ,,'P4/MCC   ,
-   'P4/MMM  ,,'P4/MNC   ,,'P4/NBMS  ,,'P4/NBMZ  ,,'P4/NCCS  ,
-   'P4/NCCZ  ,,'P4/NMM   ,,'P4/NMMS  ,,'P4/NMMS1 ,,'P4/NMMT  ,
-   'P4/NMMZ  ,,'P4/NNCS  ,,'P4/NNCZ  ,,'P4/NNCZ1 ,,'P4/NS    ,
-   'P4/NS1   ,,'P4/NZ    ,,'P4/NBM   ,,'P4/NCC   ,,'P4/NMM   ,
-   'P4/NNC   ,,'P4/N    '/
DATA (HP46(I),I=1,74)  //P4BM     ,,'P4CC     ,,'P4MM    ,
-   'P41     ,,'P41212   ,,'P4122    ,,'P4132    ,,'P42      ,
-   'P42/M   ,,'P42/MBC  ,,'P42/MCM  ,,'P42/MMC  ,,'P42/MMCS ,
-   'P42/MNM ,,'P42/NBCS ,,'P42/NBCZ ,,'P42/NCMS ,,'P42/NCMZ ,
-   'P42/NMCS ,,'P42/NMCZ ,,'P42/NNMS ,,'P42/NNMZ ,,'P42/NS   ,
-   'P42/NS1  ,,'P42/NZ   ,,'P42BC    ,,'P42MC   ,,'P42NM   ,
-   'P4212   ,,'P422     ,,'P42212   ,,'P4232    ,,'P43      ,
-   'P432    ,,'P43212   ,,'P4322    ,,'P4332    ,,'P6       ,
-   'P6-     ,,'P6-C2    ,,'P6-M2    ,,'P6-2C    ,,'P6-2M   ,
-   'P6/M    ,,'P6/MCC   ,,'P6/MCCS  ,,'P6/MMM   ,,'P6CC    ,
-   'P61     ,,'P6122   ,,'P62      ,,'P622    ,,'P6222   ,
-   'P63     ,,'P63/M    ,,'P63/MCM  ,,'P63/MCMS ,,'P63/MMC  ,
-   'P63CM   ,,'P63MC   ,,'P63MCS  ,,'P6322   ,,'P6422   ,
-   'P65     ,,'P42/N    ,,'P42/NBC  ,,'P42/NCM  ,,'P42/NMC  ,
-   'P42/NNM  ,,'P42CM   ,,'P4222   ,,'P6MM    ,,'P64     ,
-   'P6522   '/
DATA (HR(I),I=1,28)   //R3-CR   ,,'R3-CRS  ,,'R3-MR   ,
-   'R3-MRS  ,,'R3-R    ,,'R3CR   ,,'R3MR   ,,'R3R     ,
-   'R32R   ,,'R3      ,,'R3-    ,,'R3-M    ,,'R3C     ,
-   'R3M    ,,'R32    ,
-   'R3-CH   ,,'R3-H    ,,'R3-MH   ,,'R3CH   ,,'R3H     ,
-   'R3MH   ,,'R32H   ,,'R3CHR  ,,'R3HR   ,,'R32HR  ,
-   'R3-HR   ,,'R3MHR  ,,'R3-MHR '/
DATA (IS1(I),I=1,55) /41,64,67,39,64,67,63,40,63,38,2,9,9,8,15, 00017900
-   12,15,15,12,5,35,36,36,20,21,15,15,41,64,63,36,64,64,67, 00018000
-   63,63,65,38,2,9,8,5,15,15,12,5,12,41,40,38,20,9,8,15,9/ 00018100
DATA (IS2(I),I=1,41) /9,68,66,37,64,64,63,36,41,40,8,64,63,36,67, 00018200
-   65,35,39,38,1,2,9,8,15,15,12,5,5,15,12,41,40,38,21,20,20,113,00018300
-   117,124,90,68/ 00018400
DATA (IS3(I),I=1,43) /70,70,43,43,43,228,227,227,203,203,227, 00018500
-   227,203,69,42,42,202,202,226,225,226,225,1,2,43,22,196,122, 00018600
-   216,216,139,141,210,209,228,228,227,203,228,228,228,227/ 00018700
DATA (IS4(I),I=1,76) /206,206,230,230,72,72,45,73,74,46,72,72,74, 00018800
-   74,46,74,74,71,44,44,204,229,229,1,2,13,46,46,24,199,23,197, 00018900
-   79,82,120,119,122,122,121,220,217,87,140,140,139,108,107,80, 00019000
-   142,142,141,141,141,88,88,88,110,109,98,214,97,211,204,13, 00019100
-   88,142,141,214,5,15,9,5,15,12,9,8/ 00019200
DATA (IS5(I),I=1,46) /205,205,55,50,50,32,61,54,57,60,29,29,57,51,00019300

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-      53,53,28,60,56,62,62,52,33,30,29,26,7,61,57,60,29,29,54,49, 00019400
-      56,55,57,62,60,60,53,30,29,33,7,27/ 00019500
- DATA (IS6(I),I=1,86) /57,51,53,28,57,55,51,62,62,62,62,26,51,51, 00019600
-      47,59,59,25,53,62,62,59,59,59,58,31,31,28,25,26,31,31, 00019700
-      200,221,223,221,223,56,60,62,62,52,52,33,60,53,52,30,62,59, 00019800
-      59,59,58,31,52,58,48,34,30,34,33,31,31,224,224,222,201,201,6,00019900
-      6,6,59,200,48,48,224,222,201,224,224,224,222,222,222,3/ 00020000
- DATA (IS7(I),I=1,78) /1,2,7,7,6,7,7,6,3,13,13,10,10,4,14,14,11,14,00020100
-      13,13,13,10,3,14,14,14,14,11,11,14,4,13,28,25,25,34,14,14,14,00020200
-      11,14,29,26,29,33,33,26,31,31,33,31,18,19,19,18,198,17,18,16,00020300
-      17,195,3,13,10,10,10,3,3,4,11,11,14,4,4,13,7,13,7/ 00020400
- DATA (IS8(I),I=1,60) /143,147,165,164,163,163,162,158,156,144,159,00020500
-      157,151,151,149,152,152,145,150,153,154,154,75,81,117,117, 00020600
-      116,115,118,112,111,114,113,215,218,83,127,124,123,128,125, 00020700
-      125,130,130,129,129,129,129,129,126,126,126,85,85,85,125,130,00020800
-      129,126,85/ 00020900
- DATA (IS9(I),I=1,74) /100,103,99,76,92,91,213,77,84,135,132,131, 00021000
-      131,136,133,133,138,138,137,137,134,134,86,86,86,106,105,102,00021100
-      90,89,94,208,78,207,96,95,212,168,174,188,187,190,189,175, 00021200
-      192,192,191,184,169,178,171,177,180,173,176,193,193,194,185, 00021300
-      186,186,182,181,170,86,133,138,137,134,101,93,183,172,179/ 00021400
- DATA (IS10(I),I=1,28) /167,167,166,166,148,161,160,146,155,146, 00021500
-      148,166,161,160,155,167,148,166,161,146,160,155,161,146,155, 00021600
-      148,160,166/ 00021700
*          00021800
    IF(SGR(:1).EQ.'A') GOTO 10 00021900
    IF(SGR(:1).EQ.'B') GOTO 10 00022000
    IF(SGR(:1).EQ.'C') GOTO 20 00022100
    IF(SGR(:1).EQ.'F') GOTO 30 00022200
    IF(SGR(:1).EQ.'I') GOTO 40 00022300
    IF(SGR(:1).EQ.'P') GOTO 50 00022400
    IF(SGR(:1).EQ.'R') GOTO 80 00022500
    GOTO 200 00022600
*----- A AND B ----- 00022700
10 DO 11 J=1,55 00022800
  IF(SGR.EQ.HAB(J)) THEN 00022900
    ISCHEN=IS1(J) 00023000
    V='2' 00023100
    GOTO 145 00023200
  ENDIF 00023300
11 CONTINUE 00023400
  GOTO 200 00023500
*----- C ----- 00023600
20 DO 21 J=1,41 00023700
  IF(SGR.EQ.HC(J)) THEN 00023800
    ISCHEN=IS2(J) 00023900
    V='2' 00024000
    GOTO 145 00024100
  ENDIF 00024200

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21 CONTINUE                                00024300
    GOTO 200                                00024400
*----- F -----
30 DO 31 J=1,43                            00024500
    IF(SGR.EQ.HF(J)) THEN                  00024600
        ISCHEN=IS3(J)                      00024700
        V='4'
        GOTO 145                           00024800
    ENDIF                                     00024900
31 CONTINUE                                00025000
    GOTO 200                                00025100
*----- I -----
40 DO 41 J=1,76                            00025200
    IF(SGR.EQ.HI(J)) THEN                  00025300
        ISCHEN=IS4(J)                      00025400
        V='2'
        GOTO 145                           00025500
    ENDIF                                     00025600
41 CONTINUE                                00025700
    GOTO 200                                00025800
*----- P -----
50 V='1'
    IF(SGR(2:2).LT.'M') GOTO 55          00025900
    IF(SGR(2:2).LT.'0') GOTO 60          00026000
    IF(SGR(2:2).LT.'3') GOTO 65          00026100
    IF(SGR(2:3).LE.'4/') GOTO 70          00026200
    GOTO 75                                 00026300
*----- PC -----
55 DO 56 J=1,46                            00026400
    IF(SGR.EQ.HPM1(J)) THEN              00026500
        ISCHEN=IS5(J)
        GOTO 145                           00026600
    ENDIF                                     00026700
56 CONTINUE                                00026800
    GOTO 200                                00026900
*----- PM -----
60 DO 61 J=1,86                            00027000
    IF(SGR.EQ.HPM2(J)) THEN              00027100
        ISCHEN=IS6(J)
        GOTO 145                           00027200
    ENDIF                                     00027300
61 CONTINUE                                00027400
    GOTO 200                                00027500
*----- P12 -----
65 DO 66 J=1,78                            00027600
    IF(SGR.EQ.HP12(J)) THEN              00027700
        ISCHEN=IS7(J)
        GOTO 145                           00027800
    ENDIF                                     00027900

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66 CONTINUE                               00029200
   GOTO 200                                00029300
*----- P34 -----
70 DO 71 J=1,60                           00029400
   IF(SGR.EQ.HP34(J)) THEN                00029500
      ISCHEN=IS8(J)                         00029600
      GOTO 145                                00029700
   ENDIF                                     00029800
71 CONTINUE                               00029900
   GOTO 200                                00030000
*----- P46 -----
75 DO 76 J=1,74                           00030100
   IF(SGR.EQ.HP46(J)) THEN                00030200
      ISCHEN=IS9(J)                         00030300
      GOTO 145                                00030400
   ENDIF                                     00030500
76 CONTINUE                               00030600
   GOTO 200                                00030700
*----- R -----
80 DO 81 J=1,28                           00030800
   IF(SGR.EQ.HR(J)) THEN                00030900
      ISCHEN=IS10(J)                        00031000
      IF(J.LE.15) THEN                      00031100
         V='1'                                00031200
      ELSE                                    00031300
         V='3'                                00031400
      ENDIF                                   00031500
      GOTO 145                                00031600
   ENDIF                                     00031700
81 CONTINUE                               00031800
   GOTO 200                                00031900
145 CALL CONV2(ISCHEN,SGR)               00032000
200 RETURN                                00032100
   END
*****                                         00032200
*                                         * 00032300
*****                                         00032400
*                                         * 00032500
*****                                         00032600
*                                         * 00032700
*****                                         00032800
SUBROUTINE CONV2(ISC,SGR)                00032900
CHARACTER*10 SGR                         00033000
CHARACTER*6 SCH(230),SCH1(46),SCH2(52),SCH3(44),SCH4(44),SCH5(44) 00033100
EQUIVALENCE (SCH1(1),SCH(1)),(SCH2(1),SCH(47)),(SCH3(1),SCH(99)), 00033200
-          (SCH4(1),SCH(143)),(SCH5(1),SCH(187))           00033300
DATA (SCH1(I),I=1,46) /'C1 -1 ','CI -1 ','C2 -1 ',
-          'C2 -2 ','C2 -3 ','CS -1 ','CS -2 ','CS -3 ','CS -4 ',
-          'C2H-1 ','C2H-2 ','C2H-3 ','C2H-4 ','C2H-5 ','C2H-6 ',
-          'D2 -1 ','D2 -2 ','D2 -3 ','D2 -4 ','D2 -5 ','D2 -6 ',
-          'D2 -7 ','D2 -8 ','D2 -9 ','C2V-1 ','C2V-2 ','C2V-3 ',
-          'C2V-4 ','C2V-5 ','C2V-6 ','C2V-7 ','C2V-8 ','C2V-9 ',
-          'C2V-10','C2V-11','C2V-12','C2V-13','C2V-14','C2V-15', 00033400
-          'C2V-16','C2V-17','C2V-18','C2V-19','C2V-20','C2V-21', 00033500
-          'C2V-22','C2V-23','C2V-24','C2V-25','C2V-26','C2V-27', 00033600
-          'C2V-28','C2V-29','C2V-30','C2V-31','C2V-32','C2V-33', 00033700
-          'C2V-34','C2V-35','C2V-36','C2V-37','C2V-38','C2V-39', 00033800
-          'C2V-40','C2V-41','C2V-42','C2V-43','C2V-44','C2V-45', 00033900
-          'C2V-46','C2V-47','C2V-48','C2V-49','C2V-50','C2V-51', 00034000

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-      'C2V-16','C2V-17','C2V-18','C2V-19','C2V-20','C2V-21',    00034100
-      'C2V-22'/
DATA (SCH2(I),I=1,52) /'D2H-1 ','D2H-2 ','D2H-3 ','D2H-4 ',
-      'D2H-5 ','D2H-6 ','D2H-7 ','D2H-8 ','D2H-9 ','D2H-10',
-      'D2H-11','D2H-12','D2H-13','D2H-14','D2H-15','D2H-16',
-      'D2H-17','D2H-18','D2H-19','D2H-20','D2H-21','D2H-22',
-      'D2H-23','D2H-24','D2H-25','D2H-26','D2H-27','D2H-28',
-      'C4 -1 ','C4 -2 ','C4 -3 ','C4 -4 ','C4 -5 ','C4 -6 ',
-      'S4 -1 ','S4 -2 ','C4H-1 ','C4H-2 ','C4H-3 ','C4H-4 ',
-      'C4H-5 ','C4H-6 ','D4 -1 ','D4 -2 ','D4 -3 ','D4 -4 ',
-      'D4 -5 ','D4 -6 ','D4 -7 ','D4 -8 ','D4 -9 ','D4 -10'/
DATA (SCH3(I),I=1,44) /'C4V-1 ','C4V-2 ','C4V-3 ','C4V-4 ',
-      'C4V-5 ','C4V-6 ','C4V-7 ','C4V-8 ','C4V-9 ','C4V-10',
-      'C4V-11','C4V-12','D2D-1 ','D2D-2 ','D2D-3 ','D2D-4 ',
-      'D2D-5 ','D2D-6 ','D2D-7 ','D2D-8 ','D2D-9 ','D2D-10',
-      'D2D-11','D2D-12','D4H-1 ','D4H-2 ','D4H-3 ','D4H-4 ',
-      'D4H-5 ','D4H-6 ','D4H-7 ','D4H-8 ','D4H-9 ','D4H-10',
-      'D4H-11','D4H-12','D4H-13','D4H-14','D4H-15','D4H-16',
-      'D4H-17','D4H-18','D4H-19','D4H-20'/
DATA (SCH4(I),I=1,44) /'C3 -1 ','C3 -2 ','C3 -3 ','C3 -4 ',
-      'C3I-1 ','C3I-2 ','D3 -1 ','D3 -2 ','D3 -3 ','D3 -4 ',
-      'D3 -5 ','D3 -6 ','D3 -7 ','C3V-1 ','C3V-2 ','C3V-3 ',
-      'C3V-4 ','C3V-5 ','C3V-6 ','D3D-1 ','D3D-2 ','D3D-3 ',
-      'D3D-4 ','D3D-5 ','D3D-6 ','C6 -1 ','C6 -2 ','C6 -3 ',
-      'C6 -4 ','C6 -5 ','C6 -6 ','C3H-1 ','C6H-1 ','C6H-2 ',
-      'D6 -1 ','D6 -2 ','D6 -3 ','D6 -4 ','D6 -5 ','D6 -6 ',
-      'C6V-1 ','C6V-2 ','C6V-3 ','C6V-4'/
DATA (SCH5(I),I=1,44) /'D3H-1 ','D3H-2 ','D3H-3 ','D3H-4 ',
-      'D6H-1 ','D6H-2 ','D6H-3 ','D6H-4 ','T -1 ','T -2 ',
-      'T -3 ','T -4 ','T -5 ','TH -1 ','TH -2 ','TH -3 ',
-      'TH -4 ','TH -5 ','TH -6 ','TH -7 ','O -1 ','O -2 ',
-      'O -3 ','O -4 ','O -5 ','O -6 ','O -7 ','O -8 ',
-      'TD -1 ','TD -2 ','TD -3 ','TD -4 ','TD -5 ','TD -6 ',
-      'OH -1 ','OH -2 ','OH -3 ','OH -4 ','OH -5 ','OH -6 ',
-      'OH -7 ','OH -8 ','OH -9 ','OH -10'/
*****
SGR=SCH(ISC)                                00037600
90 RETURN                                     00037700
END                                         00037800
                                         00037900

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## 5.2 ITOH4XC.SGRL.FORT(INORDEF4)

```
*****
*                                         00000100
*                                         * 00000200
*      DEFINE THE REPRESENTATIVE DATA OF ICSD      * 00000300
*                                         * 00000400
*                                         VER.4.1 94.04.21      * 00000500
*                                         * 00000600
*****                                         00000700
      PARAMETER (MAX=9000)                         00000800
      COMMON /COMPND/NAME(MAX),FORM(MAX),SCH(MAX)   00001100
      COMMON /CHEM/CHEMI(20,MAX),NC(MAX),CHEMIW(20) 00001200
      COMMON /UVOL/VOL(MAX)                         00001250
      COMMON /RELDT/INO(MAX,2),NCOL(12800,2)        00001300
      DIMENSION IWNO(MAX,500),NO(3)                 00001400
      REAL*8 VOL,WVOL                            00001650
      CHARACTER*80 ICSD                           00001700
      CHARACTER*10 SCH,WSCH                         00001800
      CHARACTER*64 FORM,WFORM,NAME,WNAME           00001900
      CHARACTER*18 PRS(3)                          00002000
      CHARACTER*2 CHEMI,CHEMIW                     00002100
      CHARACTER*1 TP                             00002200
      DATA TP/' '/                                00002300
*
*                                         00002400
*      READ THE PARAMETER:DIFF1 AND DIFF2          00002465
      READ(12,* ,END=9000) DIFF1,DIFF2            00002470
*
*      READ FILE(@DATANO.DATA):READ THE NUMBER OF OUTPUT PER COMMAND 00002500
      5 READ(12,6000,END=9000) (NO(I),PRS(I),I=1,3) 00002600
      6000 FORMAT(3(I5,A18,1X))                  00002700
*
*                                         00002800
      DO 2000 N1=1,3                            00002900
      IF(NO(N1).EQ.0) GOTO 9000                00003000
      IND=0                                     00003100
      N2=0                                      00003200
      K=0                                       00003300
*
*      READ A DATA FILE EXTRACTED FROM THE ICSD DATA          00003400
      6001 FORMAT(A80)                         00003500
      10 READ(10,6001,IOSTAT=KK,END=30) ICSD       00003600
      TP=ICSD(3:3)                           00003700
      IF(TP.EQ.'0') THEN                      00003800
      DECODE(80,6110,ICSD) ICOLCD,IENTCD     00003900
      N2=N2+1                                 00004000
      GOTO 10                                00004100
      ENDIF                                  00004200
      6110 FORMAT(8X,I6,1X,I6)                 00004300
      IF(TP.EQ.'1') THEN                      00004400
      WNAME=ICSD(9:72)                        00004500
      I1=1                                    00004600
      GOTO 10                                00004700
      ENDIF                                  00004800
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IF(TP.EQ.'4') THEN          00004900
  K=K+1
  IF(K.EQ.1) THEN          00005000
    WFORM=ICSD(9:72)
    CALL CHEMICAL(WFORM,NCW)
    I4=1
  ENDIF
  GOTO 10
ENDIF
IF(ICSD(3:4).EQ.'81') THEN 00005100
  DECODE(80,6120,ICSD) WVOL
6120 FORMAT(55X,E11.5)       00005200
  I81=1
  GOTO 10
ENDIF
IF(TP.EQ.'9') THEN          00005250
  IF(ICSD(2:2).EQ.'9') GOTO 30 00005300
  WSCH=ICSD(21:30)
  DECODE(80,6130,ICSD) IV
  WVOL=WVOL/FLOAT(IV)
6130 FORMAT(31X,I1)          00005400
  I9=1
  GOTO 10
ENDIF
GOTO 10
*      CHECK SPACE-GROUP        00005500
30 NCOL(N2,1)=ICOLCD      00005600
  NCOL(N2,2)=0
  IF(IND.EQ.0) GOTO 45
  DO 40 I=1,IND             00006400
*      COMPARE SHOENFLIES SYMBOL 00006500
  IF(WSCH.NE.SCH(I)) GOTO 40 00006600
*      COMPARE CHEMICAL FORMULA 00006700
  ICHEM=0
  DO 42 IC=1,NCW             00006900
  DO 42 JC=1,NC(I)
  IF(CHEMIW(IC).EQ.CHEMI(JC,I)) ICHEM=ICHEM+1
42 CONTINUE                  00007000
  WCH=FLOAT(ICHEM*2)/FLOAT(NC(I)+NCW)
  IF(WCH.LT.DIFF1) GOTO 40
*      COMPARE UNIT CELL VOLUME 00007200
  WV=ABS(VOL(I)-WVOL)/(VOL(I)+WVOL)
  IF(WV.GT.DIFF2) GOTO 40
  NCOL(N2,2)=INO(I,1)
  GOTO 50
40 CONTINUE                  00007300
*      WHEN A NEW DATA DOES NOT MATCH THE PREVIOUS ONE 00007350
45 IND=IND+1
  INO(IND,1)=ICOLCD         00007360
                                         00007400
                                         00007500
                                         00007600
                                         00007700
                                         00007800
                                         00007900
                                         00008000
                                         00008200
                                         00008300
                                         00008350
                                         00008400
                                         00008450
                                         00008461
                                         00008462
                                         00008463
                                         00008464
                                         00008465
                                         00008466
                                         00008467
                                         00008470
                                         00008520
                                         00008530
                                         00008570
                                         00008600
                                         00008800
                                         00008900
                                         00009000
                                         00009100

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INO(IND,2)=N2          00009200
IF(I1.EQ.1) THEN       00009300
  NAME(IND)=WNAME      00009400
  I1=0                 00009500
ENDIF                  00009600
IF(I4.EQ.1) THEN       00009700
  FORM(IND)=WFORM      00009800
  DO 47 II=1,NCW        00009850
    CHEMI(II,IND)=CHEMIW(II)
47   CONTINUE            00009870
  NC(IND)=NCW           00009880
  I4=0                 00009900
ENDIF                  00010000
IF(I9.EQ.1) THEN       00010100
  SCH(IND)=WSCH         00010200
  I9=0                 00010300
ENDIF                  00010400
IF(I81.EQ.1) VOL(IND)=WVOL 00012150
50 K=0                 00012200
  IF(N2.GE.NO(N1)) GOTO 90
  GOTO 10               00012300
  00012400
*
90 CALL SGRSORT(IND)   00012500
*  WRITE(6,*) IND       00012600
*  00012700
*  00012900
  N3=0                 00013000
  DO 100 I=1,N2         00013100
  IF(NCOL(I,2).EQ.0) THEN
    N3=N3+1              00013200
    IWNO(N3,1)=NCOL(I,1)
    K=1                 00013300
  ELSE
    GOTO 100             00013400
  ENDIF                  00013500
*
  DO 110 J=I+1,N2        00013600
  IF(NCOL(J,2).EQ.NCOL(I,1)) THEN
    K=K+1                00013700
    IWNO(N3,K)=NCOL(J,1)
  ENDIF                  00013800
110 CONTINUE             00013900
*  WRITE FILE             00014000
*  LST=INT((K-1)/10)+1   00014100
*  00014200
*  00014300
*  00014400
  110 CONTINUE             00014500
*  WRITE FILE             00014600
*  LST=INT((K-1)/10)+1   00014700
*  00014800
*  LS=(M-1)*10+1          00014900
*  LE=M*10                00015000
*  IF(LE.GT.K) LE=K        00015100
*  IF(M.EQ.1) THEN         00015200
*    WRITE(11,6005) N3,(IWNO(N3,L),L=LS,LE)
*  00015300

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      ELSE                                00015400
        WRITE(11,6006) (IWNO(N3,L),L=LS,LE)
      ENDIF                               00015500
111 CONTINUE                           00015600
100 CONTINUE                           00015700
*
      WRITE(6,6007) PRS(N1),NO(N1),N3   00015800
6005 FORMAT(I5,10(I6,1X))            00015900
6006 FORMAT(5X,10(I6,1X))           00016050
6007 FORMAT(1H ,A18,2(2X,I5))       00016100
2000 CONTINUE                           00016200
      GOTO 5                            00016350
9000 STOP                               00016400
      END                                00016500
*****
*          SORT DATA ACCORDING TO THE SPACE-GROUP      * 00016600
*****                                              00016700
*
      SUBROUTINE SGRSORT(IND)             00016800
      PARAMETER (MAX=9000)              00016900
      COMMON /COMPND/NAME(MAX),FORM(MAX),SCH(MAX)    00017000
      COMMON /CHEM/CHEMI(20,MAX),NC(MAX),CHEMIW(20)  00017100
      COMMON /UVOL/VOL(MAX)               00017200
      COMMON /RELDT/INO(MAX,2),NCOL(12800,2)         00017300
      DIMENSION MNO(12800),MWNO(MAX,2)             00017600
      REAL*8 VOL,WVOL(MAX)                 00017700
      CHARACTER*10 SCH,WSCH(MAX),WSCH2          00017750
      CHARACTER*64 FORM,WFORM(MAX),NAME,WNAME(MAX)  00017800
      CHARACTER*2 CHEMI,CHEMIW              00017900
*
      WSCH2=SCH(1)                         00018250
      DO 10 I=1,IND                      00018300
        MNO(I)=1                          00018400
10 CONTINUE                           00018500
      K=0                                 00018600
      II=1                               00018700
20 DO 30 I=II,IND                     00018800
      IF(MNO(I).EQ.1) THEN              00018900
      IF(WSCH2.EQ.SCH(I)) THEN        00019000
        K=K+1                            00019100
        WFORM(K)=FORM(I)                00019200
        WNAME(K)=NAME(I)               00019300
        WSCH(K)=SCH(I)                 00019400
        MWNO(K,1)=INO(I,1)              00019500
        MWNO(K,2)=INO(I,2)              00019600
        WVOL(K)=VOL(I)                 00019700
        MNO(I)=0                          00019800
      ENDIF                             00019900
30 ENDFIF                           00020000
      ENDIF                             00020100
      ENDIF                           00020750
      MNO(I)=0                          00020800
      ENDIF                           00020900
      ENDIF                           00021000

```

```

30 CONTINUE                                00021100
    DO 40 I=II+1,IND                      00021200
        IF(MNO(I).EQ.1) GOTO 50
40 CONTINUE                                00021300
    GOTO 60                                  00021400
50 II=I                                    00021500
    WSCH2=SCH(I)
    GOTO 20                                  00021600
60 DO 70 I=1,IND                          00021700
    NAME(I)=WNAME(I)
    FORM(I)=WFORM(I)
    SCH(I)=WSCH(I)
    INO(I,1)=MWNO(I,1)
    INO(I,2)=MWNO(I,2)
    VOL(I)=WVOL(I)
70 CONTINUE                                00021900
    RETURN                                   00022000
    END                                     00022100
*****                                         00022200
*      DIVIDE FORMULA INTO EACH CHEMICAL ELEMENT * 00022300
*****                                         00022400
SUBROUTINE CHEMICAL(WFORM,NCW)              00023050
PARAMETER (MAX=9000)                       00023100
COMMON /COMPND/NAME(MAX),FORM(MAX),SCH(MAX) 00023200
COMMON /CHEM/CHEMI(20,MAX),NC(MAX),CHEMIW(20) 00023300
COMMON /UVOL/VOL(MAX)                     00023350
COMMON /RELDT/INO(MAX,2),NCOL(12800,2)     00023350
REAL*8 VOL                                 00032500
CHARACTER*10 SCH                           00032600
CHARACTER*64 NAME,FORM,WFORM               00032700
CHARACTER*2 CHEMI,CHEMIW                 00032800
CHARACTER*1 ALPB(26)                      00032900
DATA ALPB/'A','B','C','D','E','F','G','H','I','J','K','L','M','N',00033200
1      'O','P','Q','R','S','T','U','V','W','X','Y','Z'/
*                                         00033300
*                                         00033350
    DO 5 I=1,20                            00033400
    CHEMIW(I)=' '
5 CONTINUE                                00033500
    K=0                                     00033600
    I=1                                     00033700
10 IF(I.GT.64) GOTO 60                  00033800
    DO 20 J=1,26
        IF(WFORM(I:I).EQ.ALPB(J)) GOTO 30
20 CONTINUE                                00033900
    I=I+1                                  00034000
    GOTO 10                                00034100
30 DO 40 J=1,26
        IF(WFORM(I+1:I+1).EQ.ALPB(J)) GOTO 50
40 CONTINUE                                00034200

```

K=K+1	00035500
CHEMIW(K)=' '	00035600
CHEMIW(K)=WFORM(I:I)	00035700
I=I+1	00035800
GOTO 10	00035900
50 K=K+1	00036000
CHEMIW(K)=WFORM(I:I+1)	00036100
I=I+2	00036200
GOTO 10	00036300
60 CONTINUE	00036400
NCW=K	00036500
6000 FORMAT(1H ,10A2,I4)	00036700
RETURN	00036800
END	00036900

### 5.3 ITOH4XC.SGRL.FORT(SGRDIST4)

```
*****
*                                         * 00000100
*                                         * 00000200
*      DISTRIBUTION OF THE SPACE GROUP      * 00000300
*                                         VER. 4.0 94.04.21 * 00000400
*****                                         00000500
      PARAMETER (MAX=9000)                   00000600
      CHARACTER*80 ICSD                      00000700
      CHARACTER*10 SGR(MAX),SGRH(MAX),WSGR   00000800
      CHARACTER*5 PG(33)                      00000900
      CHARACTER*18 PRS(500)                   00001000
      CHARACTER*6 SCH(MAX),SCH1(46),SCH2(52),SCH3(44),SCH4(44),SCH5(44) 00001100
      DIMENSION NSGR(MAX),NSGRH(MAX),ISCHEN(MAX),ISCHGR(33),ISCNT(MAX) 00001200
      DIMENSION KK(32,2),NCOL(MAX),NO(3)     00001300
      DIMENSION ITREC(33)                   00001400
      EQUIVALENCE (SCH1(1),SCH(1)),(SCH2(1),SCH(47)),(SCH3(1),SCH(99)), 00001500
      -          (SCH4(1),SCH(143)),(SCH5(1),SCH(187)) 00001600
      DATA (KK(I,1),I=1,32)/1,2,3,6,10,16,25,47,75,81,83,89,99,111, 00001700
      -          123,143,147,149,156,162,168,174,175,177,183, 00001800
      -          187,191,195,200,207,215,221/ 00001900
      DATA (KK(I,2),I=1,32)/1,2,5,9,15,24,46,74,80,82,88,98,110,122, 00002000
      -          142,146,148,155,161,167,173,174,176,182,186, 00002100
      -          190,194,199,206,214,220,230/ 00002200
      DATA (SCH1(I),I=1,46) /'C1 -1 ','CI -1 ','C2 -1 ',
      -          'C2 -2 ','C2 -3 ','CS -1 ','CS -2 ','CS -3 ','CS -4 ',
      -          'C2H-1 ','C2H-2 ','C2H-3 ','C2H-4 ','C2H-5 ','C2H-6 ',
      -          'D2 -1 ','D2 -2 ','D2 -3 ','D2 -4 ','D2 -5 ','D2 -6 ',
      -          'D2 -7 ','D2 -8 ','D2 -9 ','C2V-1 ','C2V-2 ','C2V-3 ',
      -          'C2V-4 ','C2V-5 ','C2V-6 ','C2V-7 ','C2V-8 ','C2V-9 ',
      -          'C2V-10','C2V-11','C2V-12','C2V-13','C2V-14','C2V-15',
      -          'C2V-16','C2V-17','C2V-18','C2V-19','C2V-20','C2V-21',
      -          'C2V-22'/ 00002800
      DATA (SCH2(I),I=1,52) /'D2H-1 ','D2H-2 ','D2H-3 ','D2H-4 ',
      -          'D2H-5 ','D2H-6 ','D2H-7 ','D2H-8 ','D2H-9 ','D2H-10',
      -          'D2H-11','D2H-12','D2H-13','D2H-14','D2H-15','D2H-16',
      -          'D2H-17','D2H-18','D2H-19','D2H-20','D2H-21','D2H-22',
      -          'D2H-23','D2H-24','D2H-25','D2H-26','D2H-27','D2H-28',
      -          'C4 -1 ','C4 -2 ','C4 -3 ','C4 -4 ','C4 -5 ','C4 -6 ',
      -          'S4 -1 ','S4 -2 ','C4H-1 ','C4H-2 ','C4H-3 ','C4H-4 ',
      -          'C4H-5 ','C4H-6 ','D4 -1 ','D4 -2 ','D4 -3 ','D4 -4 ',
      -          'D4 -5 ','D4 -6 ','D4 -7 ','D4 -8 ','D4 -9 ','D4 -10'/ 00003700
      DATA (SCH3(I),I=1,44) /'C4V-1 ','C4V-2 ','C4V-3 ','C4V-4 ',
      -          'C4V-5 ','C4V-6 ','C4V-7 ','C4V-8 ','C4V-9 ','C4V-10',
      -          'C4V-11','C4V-12','D2D-1 ','D2D-2 ','D2D-3 ','D2D-4 ',
      -          'D2D-5 ','D2D-6 ','D2D-7 ','D2D-8 ','D2D-9 ','D2D-10',
      -          'D2D-11','D2D-12','D4H-1 ','D4H-2 ','D4H-3 ','D4H-4 ',
      -          'D4H-5 ','D4H-6 ','D4H-7 ','D4H-8 ','D4H-9 ','D4H-10',
      -          'D4H-11','D4H-12','D4H-13','D4H-14','D4H-15','D4H-16',
      -          'D4H-17','D4H-18','D4H-19','D4H-20'/ 00004600
      -                                         00004700
      -                                         00004800
      -                                         00004900
      -                                         00005000
      -                                         00005100
      -                                         00005200
      -                                         00005300
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DATA (SCH4(I),I=1,44) /'C3 -1 ','C3 -2 ','C3 -3 ','C3 -4 ',          00005400
-   'C3I-1 ','C3I-2 ','D3 -1 ','D3 -2 ','D3 -3 ','D3 -4 ',          00005500
-   'D3 -5 ','D3 -6 ','D3 -7 ','C3V-1 ','C3V-2 ','C3V-3 ',          00005600
-   'C3V-4 ','C3V-5 ','C3V-6 ','D3D-1 ','D3D-2 ','D3D-3 ',          00005700
-   'D3D-4 ','D3D-5 ','D3D-6 ','C6 -1 ','C6 -2 ','C6 -3 ',          00005800
-   'C6 -4 ','C6 -5 ','C6 -6 ','C3H-1 ','C6H-1 ','C6H-2 ',          00005900
-   'D6 -1 ','D6 -2 ','D6 -3 ','D6 -4 ','D6 -5 ','D6 -6 ',          00006000
-   'C6V-1 ','C6V-2 ','C6V-3 ','C6V-4 '/                         00006100
DATA (SCH5(I),I=1,44) /'D3H-1 ','D3H-2 ','D3H-3 ','D3H-4 ',          00006200
-   'D6H-1 ','D6H-2 ','D6H-3 ','D6H-4 ','T -1 ','T -2 ',          00006300
-   'T -3 ','T -4 ','T -5 ','TH -1 ','TH -2 ','TH -3 ',          00006400
-   'TH -4 ','TH -5 ','TH -6 ','TH -7 ','O -1 ','O -2 ',          00006500
-   'O -3 ','O -4 ','O -5 ','O -6 ','O -7 ','O -8 ',          00006600
-   'TD -1 ','TD -2 ','TD -3 ','TD -4 ','TD -5 ','TD -6 ',          00006700
-   'OH -1 ','OH -2 ','OH -3 ','OH -4 ','OH -5 ','OH -6 ',          00006800
-   'OH -7 ','OH -8 ','OH -9 ','OH -10 '/                        00006900
DATA (PG(I),I=1,33) /' C1',' CI',' C2',' CS',' C2H',          00007000
-   ' D2',' C2V',' D2H',' C4',' S4',' C4H',' D4',          00007100
-   ' C4V',' D2D',' D4H',' C3',' C3I',' D3',' C3V',          00007200
-   ' D3D',' C6',' C3H',' C6H',' D6',' C6V',' D3H',          00007300
-   ' D6H',' T ',' TH',' O ',' TD',' OH',' TOTAL'/          00007400
IGRP=0                                         00007500
IGRP2=1                                         00007600
I=0                                             00007800
DO 2 J=1,33                                     00007900
ITREC(J)=0                                       00008000
2 CONTINUE                                      00008100
DO 4 CC=1,3                                     00008150
WRITE(6,6835) (PG(J),J=1+11*(CC-1),11*CC)      00008200
6835 FORMAT(1H ,11(A5,2X))                      00008300
4 CONTINUE                                      00008350
*      SKIP FIRST RECORD(@DATANO.DATA)           00008355
READ(12,* ,END=3) DUMMY                         00008360
*      READ FILE(@DATANO.DATA):READ THE NUMBER OF OUTPUT PER COMMAND 00007700
6 READ(12,5000,END=3) (NO(J),PRS(I*3+J),J=1,3)    00008400
5000 FORMAT(3(I5,A18,1X))                      00008500
DO 7 J=1,3                                     00008600
7 IF(NO(J).EQ.0) GOTO 3                         00008700
I=I+1                                           00008800
GOTO 6                                         00008900
3 IGRP=IGRP+1                                    00009000
*      INITIALIZATION OF WORKING AREAS          00009100
NREC=0                                         00009200
I=1                                             00009300
IR=0                                           00009400
J=1                                             00009500
DO 100 K=1,32                                    00009600
ISCHGR(K)=0                                     00009700
100 CONTINUE                                     00009800

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```

WSGR='          ,          00009900
DO 110 K=1,MAX          00010000
  NSGR(K)=0          00010100
  NSGRH(K)=0         00010200
  ISCHEN(K)=0        00010300
  ISCNT(K)=0         00010400
  SGR(K)='          ,          00010500
  SGRH(K)='          ,          00010600
110 CONTINUE          00010700
*      READ A COLLECTION CODE OF A REPRESENTATIVE DATA 00010800
  8 ISEQ=1          00010900
  5 READ(9,6000,END=10) NSEQ,NCOL(ISEQ)          00011000
6000 FORMAT(I5,I6)          00011100
  IF(NSEQ.LT.1) GOTO 5          00011200
  IF(NSEQ.EQ.1.AND.ISEQ.GT.1) THEN          00011300
    IGRP2=IGRP2+1          00011400
    GOTO 10          00011500
  ENDIF          00011600
  ISEQ=ISEQ+1          00011700
  GOTO 5          00011800
6001 FORMAT(A80)          00011900
  10 ISEQ=ISEQ-1          00012000
  JSEQ=0          00012100
  13 IF(JSEQ.EQ.ISEQ) GOTO 35          00012200
*      READ ICSD DATA FILE 00012300
  15 READ(10,6001,END=35) ICSD          00012400
  IF(ICSD(3:3).NE.'0') GOTO 15          00012500
*      READ A COLLECTION CODE AND A RELATIVE ENTRY CODE 00012600
  17 DECODE(80,6020,ICSD) ICOLCD,ENTCD          00012700
6020 FORMAT(8X,I6,1X,I6)          00012800
  DO 20 K=1,ISEQ          00012900
    IF(ICOLCD.EQ.NCOL(K)) GOTO 22          00013000
20 CONTINUE          00013100
  GOTO 13          00013200
  22 JSEQ=JSEQ+1          00013300
  25 READ(10,6001,END=35) ICSD          00013400
  IF(ICSD(3:3).EQ.'0') GOTO 17          00013500
*      READ A SPACE GROUP SYMBOL 00013600
  IF(ICSD(2:3).NE.' 9') GOTO 25          00013700
  IR=IR+1          00013800
  WSGR=ICSD(21:30)          00013900
*
  IF(IR.EQ.1) SGR(1)=WSGR          00014000
  NN=J          00014100
  DO 50 I=1,NN          00014200
    IF(WSGR.EQ.SGR(I)) THEN          00014300
      NSGR(I)=NSGR(I)+1          00014400
      GO TO 13          00014500
    ENDIF          00014600
          00014700

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50 CONTINUE                               00014800
  J=J+1                                 00014900
  SGR(J)=WSGR                           00015000
  NSGR(J)=1                            00015100
  GOTO 13                                00015200
*
*                                          00015300
35 CALL SGRHST(J,SGR,NSGR,SGRH,NSGRH)    00015400
  CALL SGRSORT(J,SGR,NSGR)                00015500
  DO 65 K=1,J                            00015600
  DO 60 K1=1,MAX                         00015700
  IF(SGRH(K).EQ.SCH(K1)) THEN           00015800
    ISCHEN(K)=K1                         00015900
    GO TO 65                            00016000
  ENDIF                                  00016100
60 CONTINUE                               00016200
65 CONTINUE                               00016300
*   COUNT THE NUMBER OF DATA PER POINT GROUP 00016400
70 CALL SCCNT(J,ISCHEN,ISCHGR,NSGRH,ISCNT) 00016500
  WRITE(6,6800) PRS(IGRP)                00016700
  WRITE(11,*)                            00016800
  WRITE(11,*)                            00016900
  WRITE(11,6800) PRS(IGRP)                00017000
6800 FORMAT(1H ,A18)                      00017100
  WRITE(11,*)                            00017200
  DO 40 K=1,32                           00017300
  KS=KK(K,1)                            00017400
  KE=KK(K,2)                            00017500
  KM=KE-KS+1                           00017600
  LST=INT((KM-1)/10)+1                  00017700
  DO 45 I=1,LST                         00017800
  LS=(I-1)*10+KS                        00017900
  LE=LS+9                               00018000
  IF(LE.GT.KE) LE=KE                    00018100
  WRITE(11,6840) (SCH(KC),KC=LS,LE)     00018200
  WRITE(11,6850) (ISCNT(KC),KC=LS,LE)   00018300
6840 FORMAT(1H ,10(A6,2X))               00018400
6850 FORMAT(1H ,10(I5,3X))               00018500
45 CONTINUE                               00018600
  NREC=NREC+ISCHGR(K)                  00018700
40 CONTINUE                               00018800
  ISCHGR(33)=NREC                      00018850
  WRITE(11,*)                            00018900
  DO 55 CC=1,3                           00018950
  WRITE(11,6830) (PG(J),J=1+11*(CC-1),11*CC) 00019000
  WRITE(11,6815) (ISCHGR(J),J=1+11*(CC-1),11*CC) 00019300
  WRITE(6,6810) (ISCHGR(J),J=1+11*(CC-1),11*CC) 00019310
55 CONTINUE                               00019320
6830 FORMAT(1H ,11(A5,2X))              00019350
6810 FORMAT(1H ,11(I5,2X))              00019400

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6815 FORMAT(1H ,11(I5,2X))          00019500
    DO 83 K=1,32                   00019600
        ITREC(K)=ITREC(K)+ISCHGR(K)
83 CONTINUE                         00019700
    ITREC(33)=ITREC(33)+NREC         00019900
85 IF(IGRP2.GT.IGRP) THEN           00020000
    BACKSPACE 9                     00020100
    GOTO 3                           00020200
ENDIF
90 WRITE(6,*) 'TOTAL='              00020300
    WRITE(11,*)                      00020400
    WRITE(11,*) 'TOTAL='              00020600
    DO 92 CC=1,3                     00020700
        WRITE(6,6810) (ITREC(K),K=1+11*(CC-1),11*CC) 00020750
        WRITE(11,6815) (ITREC(K),K=1+11*(CC-1),11*CC) 00020800
92 CONTINUE                         00020850
    STOP                            00020900
END
*****
*      SORT DATA WITH THE FREQUENCY      *
*****
*SUBROUTINE SGRHST(N,SGR,NSGR,SGRH,NSGRH)          00021400
PARAMETER (MAX=9000)                      00021500
CHARACTER*10 SGR(MAX),SGRH(MAX),WSGR       00021600
DIMENSION NSGR(MAX),NSGRH(MAX)            00021700
DATA WSGR/'          '/                  00021800
*
*      DO 10 I=1,N                      00021900
    NSGRH(I)=NSGR(I)                  00022100
    SGRH(I)=SGR(I)                  00022200
10 CONTINUE                         00022300
    NSGRW=0                          00022400
    K=1                            00022500
20 DO 80 J=K+1,N                    00022600
    IF(NSGRH(J).GT.NSGRH(K)) GOTO 70 00022700
    IF(NSGRH(J).LT.NSGRH(K)) GOTO 80 00022800
    IF(SGRH(J).GT.SGRH(K)) GOTO 80 00022900
70    NSGRW=NSGRH(K)                00023000
    WSGR=SGRH(K)                  00023100
    NSGRH(K)=NSGRH(J)              00023200
    SGRH(K)=SGRH(J)                00023300
    NSGRH(J)=NSGRW                00023400
    SGRH(J)=WSGR                  00023500
80 CONTINUE                         00023600
    K=K+1                          00023700
    IF(K.LT.N) GO TO 20            00023800
    RETURN                         00023900
END
*****

```

```

*      SORT SPACE GROUP WITH ITS CHARACTER          * 00024200
*****SUBROUTINE SGRSORT(N,SGR,NSGR)              * 00024300
PARAMETER (MAX=9000)                            00024400
CHARACTER*10 SGR(MAX),WSGR                   00024500
DIMENSION NSGR(MAX)                           00024600
INTEGER*4 WNSGR                           00024700
*                                         00024800
*                                         00024900
K=1                                         00025000
10 DO 80 J=K+1,N                         00025100
    IF(SGR(J).LT.SGR(K)) THEN             00025200
        WNSGR=NSGR(K)                     00025300
        WSGR=SGR(K)                      00025400
        NSGR(K)=NSGR(J)                  00025500
        SGR(K)=SGR(J)                    00025600
        NSGR(J)=WNSGR                   00025700
        SGR(J)=WSGR                     00025800
    ENDIF                               00025900
80 CONTINUE                                00026000
K=K+1                                 00026100
IF(K.LT.N) GO TO 10                      00026200
RETURN                                00026300
END                                  00026400
*****COUNT THE NUMBER OF DATA PER POINT GROUP * 00026500
*      SUBROUTINE SCCNT(N,ISCHEN,ISCHGR,NSGRH,ISCNT)  * 00026600
*****SUBROUTINE SCCNT(N,ISCHEN,ISCHGR,NSGRH,ISCNT)  * 00026700
PARAMETER (MAX=9000)                      00026800
DIMENSION ISCHEN(MAX),ISCHGR(32),NSGRH(MAX),ISCNT(MAX) 00026900
*                                         00027000
*                                         00027100
DO 200 I=1,N                           00027200
145 DO 111 II=1,MAX                     00027300
    IF(ISCHEN(I).EQ.II) THEN            00027400
        ISCNT(II)=ISCNT(II)+NSGRH(I)  00027500
        GO TO 100                      00027600
    ENDIF                               00027700
111 CONTINUE                                00027800
100 IF(ISCHEN(I).EQ.1) THEN            00027900
    ISCHGR(1)=ISCHGR(1)+NSGRH(I)      00028000
    GO TO 200                      00028100
ENDIF                               00028200
IF(ISCHEN(I).EQ.2) THEN            00028300
    ISCHGR(2)=ISCHGR(2)+NSGRH(I)      00028400
    GO TO 200                      00028500
ENDIF                               00028600
IF((ISCHEN(I).GE.3).AND.(ISCHEN(I).LE.5)) THEN 00028700
    ISCHGR(3)=ISCHGR(3)+NSGRH(I)      00028800
    GO TO 200                      00028900
ENDIF                               00029000

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IF((ISCHEN(I).GE.6).AND.(ISCHEN(I).LE.9)) THEN          00029100
  ISCHGR(4)=ISCHGR(4)+NSGRH(I)
  GO TO 200
ENDIF
IF((ISCHEN(I).GE.10).AND.(ISCHEN(I).LE.15)) THEN        00029200
  ISCHGR(5)=ISCHGR(5)+NSGRH(I)
  GO TO 200
ENDIF
IF((ISCHEN(I).GE.16).AND.(ISCHEN(I).LE.24)) THEN        00029300
  ISCHGR(6)=ISCHGR(6)+NSGRH(I)
  GO TO 200
ENDIF
IF((ISCHEN(I).GE.25).AND.(ISCHEN(I).LE.46)) THEN        00029400
  ISCHGR(7)=ISCHGR(7)+NSGRH(I)
  GO TO 200
ENDIF
IF((ISCHEN(I).GE.47).AND.(ISCHEN(I).LE.74)) THEN        00029500
  ISCHGR(8)=ISCHGR(8)+NSGRH(I)
  GO TO 200
ENDIF
IF((ISCHEN(I).GE.75).AND.(ISCHEN(I).LE.80)) THEN        00029600
  ISCHGR(9)=ISCHGR(9)+NSGRH(I)
  GO TO 200
ENDIF
IF((ISCHEN(I).GE.81).AND.(ISCHEN(I).LE.82)) THEN        00029700
  ISCHGR(10)=ISCHGR(10)+NSGRH(I)
  GO TO 200
ENDIF
IF((ISCHEN(I).GE.83).AND.(ISCHEN(I).LE.88)) THEN        00029800
  ISCHGR(11)=ISCHGR(11)+NSGRH(I)
  GO TO 200
ENDIF
IF((ISCHEN(I).GE.89).AND.(ISCHEN(I).LE.98)) THEN        00029900
  ISCHGR(12)=ISCHGR(12)+NSGRH(I)
  GO TO 200
ENDIF
IF((ISCHEN(I).GE.99).AND.(ISCHEN(I).LE.110)) THEN       00030000
  ISCHGR(13)=ISCHGR(13)+NSGRH(I)
  GO TO 200
ENDIF
IF((ISCHEN(I).GE.111).AND.(ISCHEN(I).LE.122)) THEN       00030100
  ISCHGR(14)=ISCHGR(14)+NSGRH(I)
  GO TO 200
ENDIF
IF((ISCHEN(I).GE.123).AND.(ISCHEN(I).LE.142)) THEN       00030200
  ISCHGR(15)=ISCHGR(15)+NSGRH(I)
  GO TO 200
ENDIF
IF((ISCHEN(I).GE.143).AND.(ISCHEN(I).LE.146)) THEN       00030300
  ISCHGR(16)=ISCHGR(16)+NSGRH(I)
  GO TO 200
ENDIF

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        ISCHGR(16)=ISCHGR(16)+NSGRH(I)          00034000
        GO TO 200                                00034100
ENDIF                                         00034200
IF((ISCHEN(I).GE.147).AND.(ISCHEN(I).LE.148)) THEN 00034300
    ISCHGR(17)=ISCHGR(17)+NSGRH(I)          00034400
    GO TO 200                                00034500
ENDIF                                         00034600
IF((ISCHEN(I).GE.149).AND.(ISCHEN(I).LE.155)) THEN 00034700
    ISCHGR(18)=ISCHGR(18)+NSGRH(I)          00034800
    GO TO 200                                00034900
ENDIF                                         00035000
IF((ISCHEN(I).GE.156).AND.(ISCHEN(I).LE.161)) THEN 00035100
    ISCHGR(19)=ISCHGR(19)+NSGRH(I)          00035200
    GO TO 200                                00035300
ENDIF                                         00035400
IF((ISCHEN(I).GE.162).AND.(ISCHEN(I).LE.167)) THEN 00035500
    ISCHGR(20)=ISCHGR(20)+NSGRH(I)          00035600
    GO TO 200                                00035700
ENDIF                                         00035800
IF((ISCHEN(I).GE.168).AND.(ISCHEN(I).LE.173)) THEN 00035900
    ISCHGR(21)=ISCHGR(21)+NSGRH(I)          00036000
    GO TO 200                                00036100
ENDIF                                         00036200
IF(ISCHEN(I).EQ.174) THEN                      00036300
    ISCHGR(22)=ISCHGR(22)+NSGRH(I)          00036400
    GO TO 200                                00036500
ENDIF                                         00036600
IF((ISCHEN(I).GE.175).AND.(ISCHEN(I).LE.176)) THEN 00036700
    ISCHGR(23)=ISCHGR(23)+NSGRH(I)          00036800
    GO TO 200                                00036900
ENDIF                                         00037000
IF((ISCHEN(I).GE.177).AND.(ISCHEN(I).LE.182)) THEN 00037100
    ISCHGR(24)=ISCHGR(24)+NSGRH(I)          00037200
    GO TO 200                                00037300
ENDIF                                         00037400
IF((ISCHEN(I).GE.183).AND.(ISCHEN(I).LE.186)) THEN 00037500
    ISCHGR(25)=ISCHGR(25)+NSGRH(I)          00037600
    GO TO 200                                00037700
ENDIF                                         00037800
IF((ISCHEN(I).GE.187).AND.(ISCHEN(I).LE.190)) THEN 00037900
    ISCHGR(26)=ISCHGR(26)+NSGRH(I)          00038000
    GO TO 200                                00038100
ENDIF                                         00038200
IF((ISCHEN(I).GE.191).AND.(ISCHEN(I).LE.194)) THEN 00038300
    ISCHGR(27)=ISCHGR(27)+NSGRH(I)          00038400
    GO TO 200                                00038500
ENDIF                                         00038600
IF((ISCHEN(I).GE.195).AND.(ISCHEN(I).LE.199)) THEN 00038700
    ISCHGR(28)=ISCHGR(28)+NSGRH(I)          00038800

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GO TO 200	00038900
ENDIF	00039000
IF((ISCHEN(I).GE.200).AND.(ISCHEN(I).LE.206)) THEN	00039100
ISCHGR(29)=ISCHGR(29)+NSGRH(I)	00039200
GO TO 200	00039300
ENDIF	00039400
IF((ISCHEN(I).GE.207).AND.(ISCHEN(I).LE.214)) THEN	00039500
ISCHGR(30)=ISCHGR(30)+NSGRH(I)	00039600
GO TO 200	00039700
ENDIF	00039800
IF((ISCHEN(I).GE.215).AND.(ISCHEN(I).LE.220)) THEN	00039900
ISCHGR(31)=ISCHGR(31)+NSGRH(I)	00040000
GO TO 200	00040100
ENDIF	00040200
IF((ISCHEN(I).GE.221).AND.(ISCHEN(I).LE.230)) THEN	00040300
ISCHGR(32)=ISCHGR(32)+NSGRH(I)	00040400
GO TO 200	00040500
ENDIF	00040600
200 CONTINUE	00040700
RETURN	00040800
END	00040900

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