

From: PALRES::BOWLUS "Steve Bowlus" 21-MAR-1994 13:11:22.44
To: SNDZEH:"toukie@zui.unizh.ch"
CC: BOWLUS
Subj: Sterimol query

Sorry to be so late to respond: I was at the ACS national meeting all last week.

I modified my cymene structure to a sec-butyl toluene, and encountered no problems. When I used the torsion values you list, however, I got the same math error you did. There was also a message in the output file about failure of the LOAD(CON) module, or some such nonsense. I was able to fix the problem by 1) making sure there is a space between consecutive values of the torsion angles (even if this is a violation of the format; modern FORTRANS can usually read "free format" in which values are delimited by spaces) or 2) truncating/rounding the torsions at two decimal places so there is a space. Looking at the output, STERIMOL appears to be reading only the first two decimals anyway (I think the format is F6.2, which would limit the precision). This truncation/rounding is not a problem for your calculation; even a single decimal is probably not physically significant. Certainly three is excessive; after all, you are inputting 3 to 5 sig figs to get a result which is (at best) three. So just input the first two decimals, and make sure there is a space between the numbers.

The reversals of the values for B 1-4 has to do with the definition of the variables, the assumed orientation of the ring, and the assumed sense of direction as one traces the path. This is the point that Hoogenstraaten is addressing in his letter to Plummer. Because some of these things can be only poorly defined (especially as you move from one platform to another), the "early Bs" are not advocated as descriptors. IF you have a visualization program so that you can assure yourself that the program is aligning molecules in the same fashion, you could probably generate an internally consistent data set. But I would not hold my breath. In all events, I would consider only L and B5 reliable, and perhaps take the risk that B1 was the smallest value in the set B1 to B4 if the definitions are consistent with B1 always being the smallest (I have always used only L and B5 myself, rather than worry about the fine structure).

Hope this helps,
sb

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Dr. E.L. Plummer,
FMC Corp., Agricultural Chem.Div
100 Niagara Street,
MIDDLEPORT, N.Y. 14105

U.S.A.

your ref.
our ref.
dept.
date

agro biological laboratory 'boekesteyn'

March, 1979

Dear dr Plummer,

As one of the persons who have requested our STERIMOL program, you will probably be interested in some additional documentation on this subject.

In the first place, we found it necessary to introduce the possibility of formulating "special" atoms in the input, i.e. atoms which do not belong to the standard list of programmed atoms. Some examples are mentioned in the accompanying paper. Our published parameters of substituents like cyclobutyl or cyclopentyl were partly calculated "by hand", partly by the program with incorrect atoms, and I fear that some of those data are wrong.

Further, in recalculating some of our parameters, you may have found values of B_2 , B_3 and B_4 that differ from our published values. The reason is the following: for a number of substituents, the minimum width (B_1) does not occur at one singular orientation, but a continuous range of orientations of the group while turning around the bond axis. Hence, the orientation at which the minimum is found - and where the values of B_2 , B_3 , and B_4 are calculated - will depend on the programming, the starting position and the sense of rotation. Since we have made some alterations to the program at this point after finishing our original calculations, the minimum width B_1 , although with unchanged value, may sometimes occur at a different point of the molecular projection, with different values of the other B-parameters as a consequence.

In view of their uncertain definition and their questionable value both from the theoretical and the practical point of view, we have decided to refrain from using the width parameters B_2 - B_4 . Instead, the parameter B_1 , representing the real maximum width, appears to us - beside L and B_1 - a useful steric parameter.

Yours sincerely,

- one enclosure-

(Dr. W. Hoogenstraaten)

BR

STERIMOL for the PC

Calculation of Verloop's STERIMOL Parameters

Based on the program STERIMOL by W. Hoogenstraaten
Duphar B.V., the Netherlands

Converted for the IBM PC by Stephen Bowlus
Sandoz Crop Protection Corp.
Palo Alto, California

The enclosed diskette contains source code and executable files for STERIMOL, the program developed for estimation of the Verloop steric parameters for QSAR. The original program was written by Verloop and Hoogenstraaten at Duphar B.V. This went through several revisions (see comments in the file STERIMOL.SRC). This PC version is based on the program obtained from E. L. Plummer at FMC Ag Chem.

The FORTRAN code for the PC has been somewhat cleaned up, to remove many references and explanations of the generations of changes that were made, except where these were deemed important to understanding the current version of the program. If the history of the source code is of importance or interest, the file STERIMOL.SRC contains the unconverted VAX version of the program. Rather than clutter up the code with (more) extraneous remarks, notes on the conversion are appended to the documentation.

INSTALLATION and OPERATION

The distribution diskette contains the following files:

CONVERT.DOC -- This message.
STERIMOL.SRC -- VAX source code, from which this program was written.
STERIMOL.FOR -- Source code for MicroSoft FORTRAN, v. 3.31 or 5.0.
STERIMOL.EXE -- Executable image, compiled under FORTRAN 5.0 for the 80286 or 80386 with math coprocessor.
STERIMOL.52I -- Executable image, compiled under FORTRAN 5.0 for the 80286 or 80386 using coprocessor emulation (coprocessor optional).
STERIMOL.50I -- Executable image, compiled under FORTRAN 5.0 for the 8086 using coprocessor emulation.
STERIMOL.331 -- Executable image, compiled under FORTRAN 3.31, using the default math library (coprocessor not used).
EXAMPLE.INP -- Sample input deck
EXAMPLE.OUT -- Sample results file.

To install the program on a hard disk, copy the files STERIMOL.-EXE (or other executable file, renaming if necessary) and EXAMPLE.INP to an appropriate directory.

The input file, EXAMPLE.INP is edited with any ASCII text editor for the compound and radicals (fragments) of interest. The rules for formula notation, written by Hoogenstraaten, are given in the following section. For the remainder of the file, note the following, taken from the program listing:

```
C ***** INPUT CARDS *****
C THE FIRST CARD CONTAINS THE 33 USED SYMBOLS; STARTING WITH 1 IN COLUMN
C 1. SYMBOL NR 27 IS A SPACE.
C 1234567890ABCDEFHINOPRSTXZ (&*),=
```

- This line no longer appears in the input file. This data declaration is now in the body of the program. This line should be not be included in any test file based on Hoogenstraaten's examples in the following section of the documentation.

```
C NEXT FOLLOW (IF WANTED) THE FORMULAE FOR THE 'RADICALS', OF THE
C FOLLOWING GENERAL TYPE:
C ZKK=FORMULA*
C WHERE KK IS A TWO-DIGIT INTEGER NUMBER (01 - 99). A RADICAL MAY BE ANY
C SYMBOL STRING WHICH IS PART OF A VALID FORMULA. IF NECESSARY, IT MAY BE
C CONTINUED LIKE A FORMULA CARD. CLOSE OR REPLACE THE RADICAL-CARD SET BY
C A BLANK CARD.
C FOR EACH MOLECULE THE FOLLOWING CARDS ARE GIVEN:
C (1) THE INTEGER IPR (I4): THE OUTPUT INDEX (1 OR 2);
C (2) THE FORMULA. IF ONE CARD IS NOT SUFFICIENT, END THIS CARD WITH A
C & SIGN AND CONTINUE ON THE NEXT CARD.
C (3) NUMBER OF THE TORSION ANGLES (I4). IF NONE ARE TO BE GIVEN, REPLACE
C THIS CARD BY A BLANK ONE.
C (4) THE TORSION ANGLES (IX,F7.2); DECIMAL POINTS AT COLUMNS 6, 14, 22,
C ....).
C AFTER THE SETS OF MOLECULE-INPUT CARDS: ONE BLANK CARD.
```

- Only one molecule may be processed in each input file. Input files may be chained in a DOS .BAT file, if a number of molecules or conformers are being considered.

The command is then given:

```
C:\> STERIMOL < STERIMOL.INP
```

or

```
C:\> STERIMOL < STERIMOL.INP > STERIMOL.OUT
```

In the first command, all output will be displayed on the screen.

With the second command, all output will be written to the file, STERIMOL.-OUT, without screen echo. Since the screen scrolls very fast (too fast to read much of the output), the second command is preferred. Alternatively, the output can be directed to an attached printer (> PRN:).

For the FORTRAN v. 3.31 version of the program, rather than use DOS redirection, the program will prompt you for Unit 5 and Unit 6. File names for input and output, respectively, should be given at the prompts.

The input and output files may have any legal DOS name. The extension is not required. Files can be named for the molecule being examined, for example, COMPND1.INP and COMPND1.OUT, or JUNKIN and JUNKOUT.

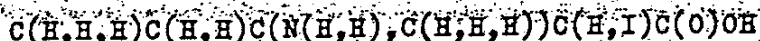
```
C ***** OUTPUT *****
C   FOR IPR = 1 :
C   THE RADICAL FORMULAE (IF PRESENT);
C   THE MOLECULE FORMULA AS IT WAS INPUT;
C   SERIAL NUMBER, NUMBER OF ATOMS, OUTPUT INDEX;
C   FULLY WRITTEN FORMULA, WITH 'TRANSLATION' OF THE RADICALS;
C   LIST OF THE TORSION ANGLES;
C   TABLE OF THE VANDERWAALS RADII AND COORDINATES OF THE ATOMS;
C   LIST OF THE STERIC PARAMETERS: L; B(1) - B(4) AND B(5) (MAXIMUM WIDTH);
C   A WARNING IF NEIGHBOURING ATOMS HAVE OVERLAPPING VANDERWAALS SPHERES.
C   FOR IPR = 2 IN ADDITION:
C   AN X, Y AND A Y, Z PROJECTION OF THE MOLECULE;
C   A LIST OF THE ATOMS, ORDERED BY INCREASING X COORDINATES, SERVING TO
C   RAPIDLY IDENTIFY THE PLOTTED ATOMS.
```

- The output type parameter (single digit above the structure notation) is set to 2 for a "connect-the-dots" structure representation, or to 1 for normal, numerical output. The printed structures may be meaningless, due to line wrapping. Success is more likely with a printer set to 132 columns.

Rules for formula notation

1. Chain structure

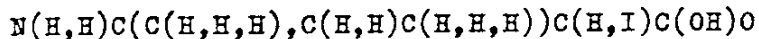
The linear chemical formula can, as a rule, be written in many ways. First one must choose a main chain of connected atoms, to which various side chains may be attached. Side chains are written between parentheses after the main-chain atom, to which they are attached; more side chains at one atom are separated by commas. Thus, a simplified formulation of the molecule of fig. 1 could be:



where the (primary) chain is taken as the atom sequence 1, 2, 3, 6, 7, 9, 10, while groups $N(4)H_2$ and $C(5)H_3$ are side chains at atom nr 3. In their turn, these side chains are secondary main chains with respect to their own side chains H.

Other side chains are the hydrogen atoms at C(1), C(2) and C(6) and the O(8) at C(7); the hydrogens bound to N(4) and C(5) can be viewed as secondary side chains.

An equally valid notation, among many others, is:



with the atoms 4, 3, 6, 7 and 8 as the primary chain, a secondary main chain being formed by atoms 2 and 1.

2. Atom types and bond types

Because many atoms have more than one bond geometry, we must indicate the bonding type. This is done by numbers written after the atomic letter symbol, e.g. C is the normal tetrahedral carbon

Table I

symbols and bond types of atoms

type nr	symbol	bond values	use
1	C	4 x 1	tetrahedral carbon
3	C2	2, 1, 1	ethylene carbon
4	C3	3, 1	acetylene carbon
5	C4	4, 2, 1	amide carbon
6	C5,N5	3, 3, 1	C (or N) in aromatic 5-ring
7	C6,N6	2, 2, 1	C (or N) in aromatic 6-ring
8	C7	3, 2, 1	carbon linking 5 and 6-ring
9	C8	2, 2, 1, 1	cyclopropane carbon
10	H	1, 5	hydrogen
11	N	4 x 1	tetrahedral nitrogen
13	C66	2, 2, 2	carbon linking two 6-rings
15	N4	5, 4, 1	amide nitrogen
20	O	1, 1	normal oxygen
22	O2	2	double bonded oxygen
23	P	4 x 1	tetrahedral phosphorus
24	S	1, 1	normal sulfur
25	S1	6 x 1	octahedral sulfur
26	F	1	fluorine
27	Cl	1	chlorine
28	S4	4 x 1	tetrahedral sulfur
29	B1	1	bromine
30	I	1	iodine

atom, while C2 and C3 stand for the ethylene and acetylene carbon atoms, respectively. Other C atoms like C5 and C6 are used in 5 or 6-membered rings; C7 links aromatic 5-rings and 6-rings together. As the use of two letters for an atomic symbol would give rise to programming complications, we have taken the combinations B1 for Br and C1 for Cl.

There are also differences between some bonds on most atoms. For instance, the double bond on C2 is different from the two single bonds. In order to discriminate between bonds with different geometrical properties, the introduction of 5 bond types (bond values) has been sufficient up till now.

There is only a superficial connection between e.g. a D bond (with bond value 2) and the double bond as known in organic chemistry, the D bond also being used for the connection between two C6 atoms (in 6-rings) or two C8 atoms (cyclopropane ring).

The bond value is indicated by a letter D, T, A, E or nothing between atomic symbols. A more complete notation for e.g. the COOH group of fig. 1 would be: C2(D02)OH.

The various atom types and the use of the bond values are given in tables I and II.

3. Rings

In order to indicate ring closures in molecules, each of the atoms that bring about a ring closure must carry the same quasi-bond partner X1, X2, etc. (up to X9 may be used). If the bond made by the two X's is one of a special type (bond value larger than 1), this should be

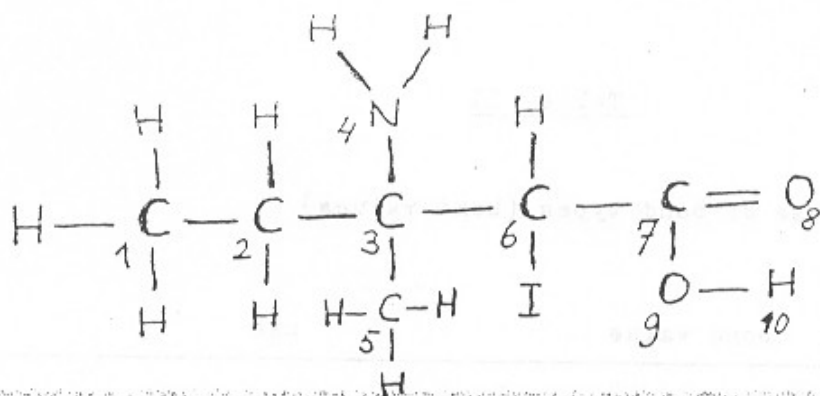


fig. 1

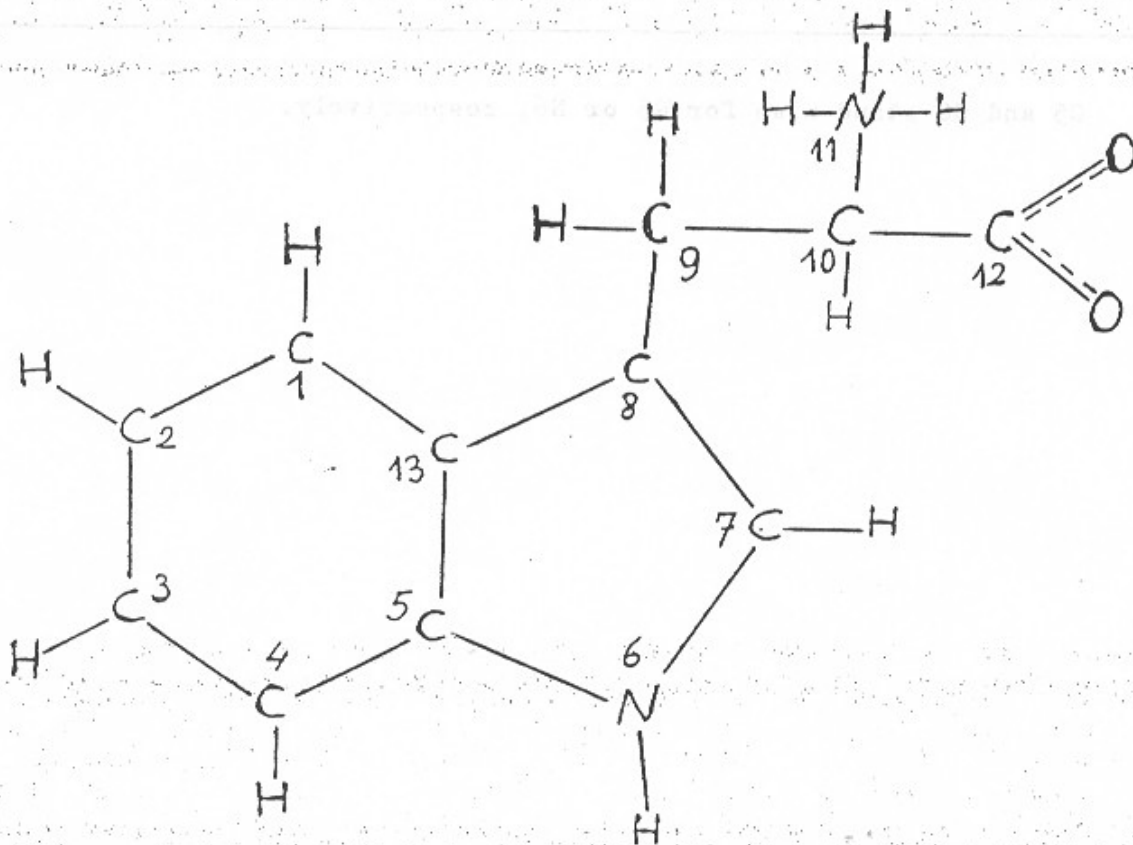


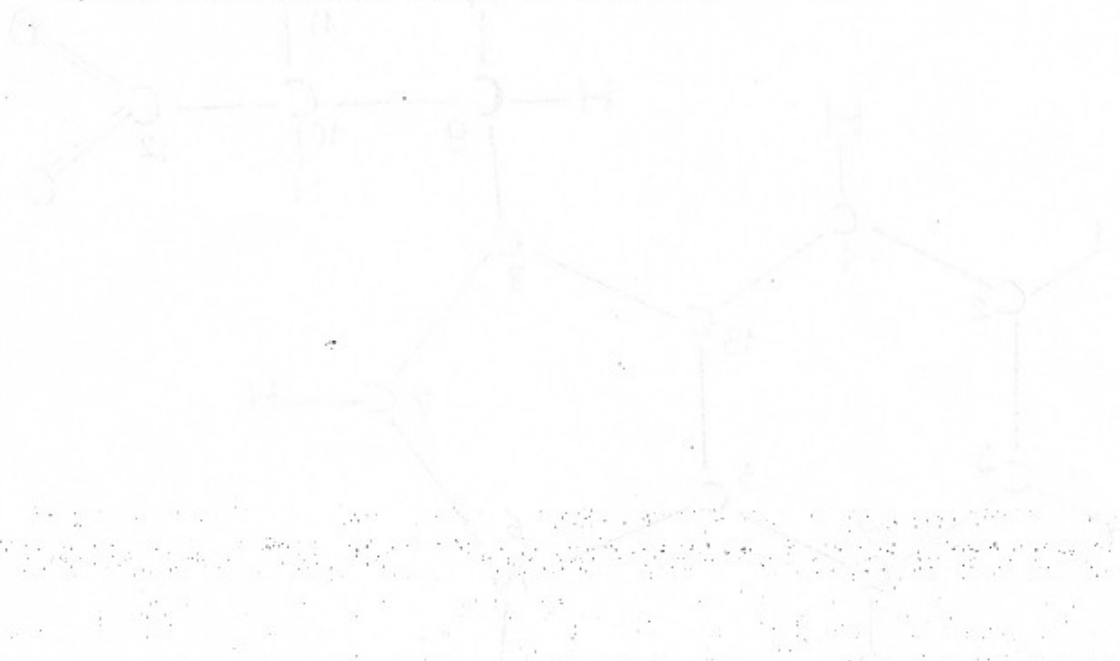
fig. 2

Table II

use of bond types (bond values)

bond-type symbol	bond value	use
none	1	all single bonds except C8-C8 and C4-N4; further C7-C7, P-O, S1-O, S4-O.
D	2	C2-C2, C2-O2, C4-O2, C6-C6, C6-C7, C8-C8, C66-C66, C6-C66 .
T	3	C3-C3, C5-C5, C5-C7 .
A	4	C4-N4 .
E	5	N4-H

C5 and C6 stand also for N5 or N6, respectively.



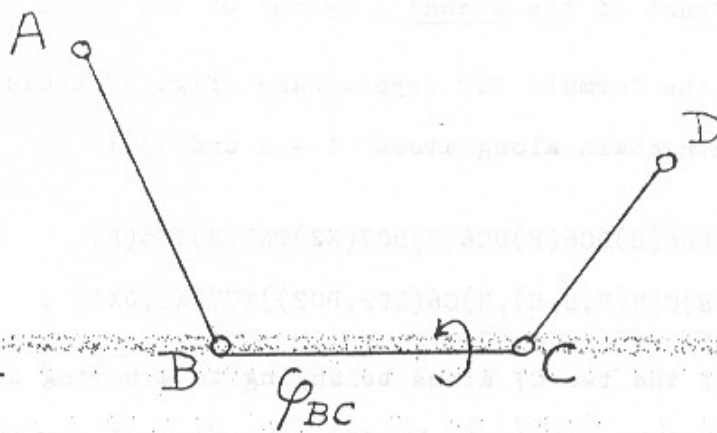


fig. 3 a

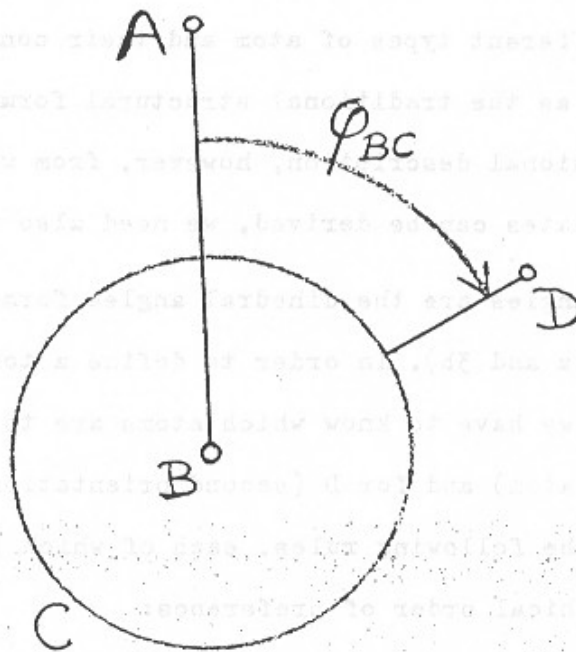
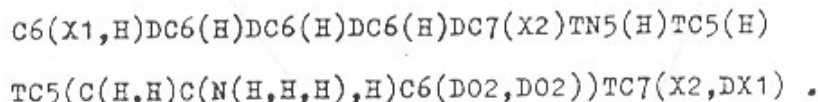


fig. 3 b

indicated in front of the second X symbol of the pair.

For instance, the formula for tryptophane (fig. 2) could be written as follows (main chain along atoms 1 - 8 and 13):



Note the use of the two C7 atoms belonging to a 6-ring and a 5-ring (these are linked by a "single bond"), the X1 used for the D bond between C(1) and C(13), and the X2 for the bond between C(5) and C(13). Incidentally, C6 with two connected "double" bonded O2 atoms is used here for the deprotonated carboxyl group.

4. Conformation angles

So far, the linearised formula describes the molecule as far as the different types of atom and their connectivity are concerned, i.e. as far as the traditional structural formula does. For a complete three-dimensional description, however, from which a unique set of atomic coordinates can be derived, we need also the torsion angles.

These angles are the dihedral angles formed by three consecutive bonds (figs 3a and 3b). In order to define a torsion angle around some bond B - C we have to know which atoms are to be taken for A (first orientation atom) and for D (second orientation atom). These atoms are chosen along the following rules, each of which is to be followed in the given hierarchical order of preference:

1. The first orientation atom of a bound atom pair is the atom, that
 - 1a. precedes the first atom of the pair in its own chain or in the major chain, to which the chain of the first atom is attached

Table III

atom pair	first orientation	second atom	rules
N(4) - C(3)	H	C(6)	1c ; 2a
C(3) - C(5)	N(4)	H	1a ; 2b
C(3) - C(2)	N(4)	C(1)	1a ; 2a
C(2) - C(1)	C(3)	H	1a ; 2b
C(3) - C(6)	N(4)	C(7)	1a ; 2a
C(6) - C(7)	C(3)	O(8)	1a ; 2b
C(7) - O(9)	C(6)	H(10)	1a ; 2a

The non-subscripted H atoms are the first H atoms bound to the atom in question.

Table IV

atom pair	first orientation	second atom	rules	
C(1) - C(2)	X1=C(13)	C(3)	1c ; 2a	0
C(2) - C(3)	C(1)	C(4)	1a ; 2a	0
C(3) - C(4)	C(2)	C(5)	1a ; 2a	0
C(4) - C(5)	C(3)	N(6)	1a ; 2a	180
C(5) - N(6)	C(4)	C(7)	1a ; 2a	180
N(6) - C(7)	C(5)	C(8)	1a ; 2a	0
C(7) - C(8)	N(6)	C(13)	1a ; 2a	0
C(8) - C(9)	C(7)	C(10)	1a ; 2a	
C(9) - C(10)	C(8)	C(12)	1a ; 2a	
C(10) - N(11)	C(9)	H	1a ; 2b	
C(10) - C(12)	C(9)	O	1a ; 2b	
C(8) - C(13)	C(7)	X2=C(5)	1a ; 2b	0

1b. follows this atom in the main chain;

1c. follows this atom as a first side-chain atom, even if this is a Xk symbol. In the latter case, the first orientation atom is the atom represented by this Xk.

2. The second orientation atom of the pair is the atom, that

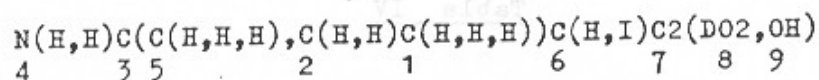
2a. follows the second atom of the pair in its own chain;

2b. follows this atom as a first side-chain atom. In case of an Xk: see rule 1c.

The notation of non-zero conformation angles is accomplished by writing the letter R in front of the second atom of the pair.^{x)} The angle values are given separately in the order of the R's in the formula.

We shall exemplify the rules with the molecules of figs 1 and 2.

For molecule nr 1 we take the following notation:



The first torsion angle encountered is that around bond N(4) - C(3).

For the first orientation atom, linked to N(4), rules 1a and 1b cannot apply (the last one not because that would give us the second atom of the pair itself); hence in accordance with rule 1c we have to take the first atom (H) bound to N.

For the second orientation atom, we can use rule 2a and obtain C(6).

In this way, one can find the various partners of dihedral angles as given in table III. For the molecule of fig. 2, formulated as in section 3, we obtain table IV.

^{x)} If an R symbol occurs together with a bond-value letter like D, the order of these symbols is immaterial.

Table IV (continued)

atom pair	first orientation	second atom	rules	
C(1) - C(13)	C(2)	X2=C(5)	1b ; 2b	0
C(5) - C(13)	C(4)	---	1a ; --	-

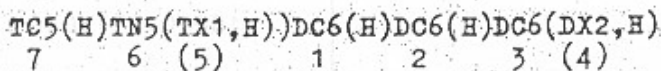
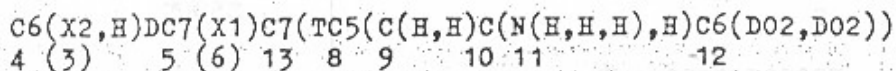
In the latter table, the last column shows the values of the torsion angles which must be taken in order to obtain the correct ring structure. In this case, we should at least indicate two conformation angles of 180° , one between C(4) and C(5) and one between C(5) and N(6), to ensure a correct ring structure. Further angles may be defined for the four bonds to and in the side chain at atom C(8).

There occurs an apparent difficulty in the last line of table IV.

Here, the second orientation atom could not be indicated because the only possibility would be C(5), which is one of the pair atoms.

However, the organization of the program makes this line and also the preceding one superfluous: the orientation of an atom is governed only by the bond with the atom with the nearest lower ranking number in the formula. Of the three bonds made by C(13), this is the bond with C(8), and accordingly the two other bonds with C(1) and C(5) can be left out of account.

The molecule could also be formulated without any non-zero conformation angles for the rings. One such possibility is:



Formally, we have here a primary chain consisting of the atoms 4, 5, 13, 1, 2, 3. Attached to this is, among others, the side chain 8, 7, 6 with a link to 5 and a subsidiary side chain 9, 10, 11, 12. The following significant dihedral quadruples can be formulated for the ring closure:

3-4-5-13, 4-5-13-1, 5-13-8-7, 5-13-1-2, 13-8-7-6, 8-7-6-5, 13-1-2-3, and 1-2-3-4, all angles being zero.

Input card deck for the output example:

1234567890ABCDEFHINOPRSTXZ. (£*), =

Z01=N6(D02,D02) *

Z02=C(H,H) *

Z03=C(H,H,H) *

Z04=C(H,RC(H,H,H))RC(H,H)RC(H,H,H) *

Z50=C(H,H)RC(H,C(H,H,H)) £

RC(H,H,H) *

continuation

11

1

HZ02RZ02C1 *

180.0

1

2

180.0

HSR £

2

Z50 *

HZ02RZ02RZ01 *

4

2

180.0 180.0 60.0 60.0

180.0 0.0

1

HZ02R202C1

MOLECULE NR. 1

NUMBER OF ATOMS = 8 OUTPUT INDEX = 1

HC(H,H)RC(H,H)C1

TORSION ANGLES: 180.00
VANDERWAALS RADII (*100) AND COORDINATES

1	100	0.0	0.0	0.0
2	150	-1.10	0.0	0.0
3	100	-1.47	0.27	-1.00
4	100	-1.47	-1.00	0.27
5	150	-1.61	1.03	1.03
6	100	-1.25	0.76	2.03
7	100	-1.25	2.03	0.76
8	180	-3.37	1.03	1.03

STERIC PARAMETERS: L= 5.57

B(1) - B(4): 1.52 3.25 1.90 1.91 R(5): 3.25

Z01=N6(002,002)

Z02=C(H,H)

Z03=C(H,H,H)

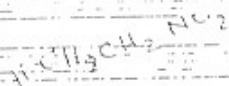
Z04=C(H,RC(H,H,H))RC(H,H)RC(H,H,H)

Z50=C(H,H)PC(H,C(H,H,H))PC(H,H,H)

MOLECULE NR 2

NUMBER OF ATOMS = 10 OUTPUT INDEX = 2

HC(H,H)RC(H,H)RN6(D02,D02)



TORSION ANGLES: 180.00 0.0
 VANDERWAALS RADII (*100) AND COORDINATES

1	100	0.0	0.0	0.0
2	150	-1.10	0.0	0.0
3	100	-1.47	0.27	-1.00
4	100	-1.47	-1.00	0.27
5	150	-1.61	1.03	1.03
6	100	-1.25	0.76	2.03
7	100	-1.25	2.03	0.76
8	170	-3.11	1.03	1.03
9	135	-3.74	0.26	0.26
10	135	-3.74	1.80	1.80

STERIC PARAMETERS: L = 5.49

B(1) - B(4): 1.52 3.89 1.90 1.91 R(5): 3.89

TAKE CARE: MUTUAL PENETRATION OF FOLLOWING ATOMS:

NRS. 2 AND 9 : OVERLAP IS 0.18

MOLECULE NR 3

NUMBER OF ATOMS = 9 OUTPUT INDEX = 1

HORS4(O,O)C(H,H,H)

TORSION ANGLES: 180.00

VANDERWAALS RADII (*100) AND COORDINATES

1	100	0.0	0.0	0.0
2	135	-0.99	0.0	0.0
3	200	-1.48	0.95	0.95
4	135	-1.01	0.60	2.26
5	135	-1.01	2.26	0.60
6	150	-3.02	0.94	0.94
7	100	-3.38	0.20	0.20
8	100	-3.39	1.94	1.94
9	100	-3.39	1.94	0.67

STERIC PARAMETERS: L= 4.92

B(1) - B(4): 1.35 3.62 1.35 3.59 B(5): 3.68

1	9	135	-3.74	0.26	0.26
2	10	135	-3.74	1.80	1.80
3	8	170	-3.11	1.03	1.03
4	5	150	-1.61	1.03	1.03
5	4	100	-1.47	-1.00	0.27
6	3	100	-1.47	0.27	-1.00
7	6	100	-1.25	0.76	2.03
8	7	100	-1.25	2.03	0.76
9	2	150	-1.10	0.0	0.0
10	1	100	0.0	0.0	0.0

MSRZ50

MOLECULE NR 4

NUMBER OF ATOMS = 15 OUTPUT INDEX = 2

HSRC (H,H) RC (H,C (H,H,H)) RC (H,H,H)

TORSION ANGLES: 180.00 180.00 60.00 60.00
VANDERWAALS RADII (*100) AND COORDINATES

1	100	0.0	0.0	0.0
2	170	-1.37	0.0	0.0
3	150	-1.81	1.24	1.24
4	100	-1.39	0.95	2.22
5	100	-1.39	2.22	0.95
6	150	-3.34	1.35	1.35
7	100	-3.76	1.64	-0.37
8	150	-3.92	-0.02	1.76
9	100	-3.10	-0.74	1.88
10	100	-4.46	0.08	2.71
11	100	-4.61	-0.38	0.98
12	150	-3.71	2.40	2.40
13	100	-3.30	3.38	2.11
14	100	-4.81	2.48	2.48
15	100	-3.30	2.11	3.38

STERIC PARAMETERS: L= 6.21

B(1) - B(4): 1.70 4.44 1.70 4.31 B(5): 4.98

TAKE CARE; MUTUAL PENETRATION OF FOLLOWING ATOMS:

NPS. 2 AND 8 ; OVERLAP IS 0.10

1	14	100	-4.61	2.48	2.48
2	11	100	-4.61	-0.38	0.98
3	10	100	-4.46	0.08	2.71
4	8	150	-3.92	-0.02	1.76
5	7	100	-3.76	1.64	0.37
6	12	150	-3.71	2.40	2.40
7	6	150	-3.34	1.35	1.35
8	15	100	-3.30	2.11	3.38
9	13	100	-3.30	3.38	2.11
10	9	100	-3.10	-0.74	1.88
11	3	150	-1.81	1.24	1.24
12	4	100	-1.39	0.95	2.22
13	5	100	-1.39	2.22	0.95
14	2	170	-1.37	0.0	0.0
15	1	100	0.0	0.0	0.0

CONVERSION NOTES

If you are really interested in this type of bumpf, the following description will probably make more sense if reviewed together with listings of STERIMOL.SRC (the original VAX code) and STERIMOL.FOR (the Microsoft FORTRAN code). While some of the corrections are serious, others were made only to stop complaints from the compiler:

The BLOCK DATA segment was altered to correct a statement out of order. The COMMON/CHAR/ declaration was moved to the top of the block. The COMMON block CHAR was redefined throughout the program to ICH(33). The DATA statement in which the characters are defined was altered so the block definition and declared data are in agreement.

The COMMON block VAR was made into a blank common block, to accommodate different definitions of this block.

The variables P and KR were removed where they were referenced but not used. (N.B. There is a surviving constant P!)

I/O unit assignments were changed. Unit 5 is the standard input (keyboard), redirected to the input file in the DOS command line when the program is started. Unit 6 is the standard output (screen) and the output file is created by DOS redirection. (Note that MS Fortran 3.31 and 5.0 handle these differently!) References to other I/O units in the program (mostly to get the VAX to write to the terminal), and unit assignments to input and output files were deleted.

All references or calls to EXIT were removed. Statement 9999 was changed from "CALL EXIT" to "CONTINUE". Conditional branches to CALL EXIT are now directed to this continuation.

The DO loops associated with statement 130 were renumbered (now 131) and the inner loop now terminating with 132 was revised, to stop complaints of using a label across blocks.