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TITLE	ISOMER - INTERACTIVE STUDY OF ORGANIC MOLECULES BY EDUCATIONAL REINFORCEMENT
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SOURCE LANGUAGE	Can be assembled by: MACRO-8 PAL-D PAL-8 PAL-10

ISOMER - INTERACTIVE STUDY OF ORGANIC MOLECULES BY EDUCATIONAL REINFORCEMENT

DECUS Program Library Write-up

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ABSTRACT

ISOMER was written to establish the utility of the small Lab-8 as a tool for computer assisted instruction. It is designed to assist students in learning organic nomenclature by asking them to identify all 21 isomers of $C_5H_{10}Br_2$. Carbon skeletons are drawn on the scope by typing C's, the position of which are controlled by Space, ↑ , ←, Line Feed and Return. The positions of the two bromines are controlled by the four Lab-8 knobs.

After the bromines are adjusted to represent a legitimate isomer, typing N produces on the Teletype:

a) the IUPAC name of that isomer, and
b) whether this student has previously identified this isomer.

When the student indicates that he has completed all of the possible isomers by typing D, the computer either congratulates or condoles him and lists any isomers which he may have omitted.

STORAGE AND LANGUAGE

ISOMER occupies locations 0-5377, and is available as a binary tape or an ASCII source tape which can be assembled using the MACRO-8, PAL-D, PAL-8 or PAL-10 assemblers.

HARDWARE

A Lab-8 computer with 4K of core. No high speed or mass storage devices are necessary.

LOADING AND USE

ISOMER is loaded using the standard Binary Loader. The starting address is 0200. All instructions for its use are typed out by the program when I is typed. A copy of these instructions and of a successful execution of the program is appended.

OPERATING SUGGESTIONS

Traps are included to prevent overlapping of carbons with each other or with bromines and to prevent overlapping of bromines with carbons, bonds, or each other. All of these errors, as well as discontinuous chains produce the message:

I'M SORRY, I CAN'T FIGURE THAT STRUCTURE OUT.

Movement of bromines with the Lab-8 knobs is quantized. They must be adjacent to the carbon to which you mean them to be attached. The program recognizes only one such position for bromines above or below the carbon, but recognizes two such positions for bromines to the left or right of carbon atoms. Bromines which are too far distant from the carbon atoms to be connected produce the error message:

NOT A LEGAL STRUCTURE

Since the display layout produces 90° bond angles, it is possible to represent isomers of dibromomethylcyclobutane. These are not, however, isomers of $C_5H_{10}Br_2$ and they produce an error message.

Typing CONTROL/C at any time produces a jump to location 7600, with the accumulator clear. This can be used to call the PS-8 or Disk System Monitors.

Logical Flow of ISOMER

The logic of the list structuring and coordinate handling is described in comments contained in the listing. Briefly, the character display is handled by packing both the x and y coordinates into one 12-bit word as XXYY. These words are unpacked to ØXXØ and ØYYØ and serve as the origin setting for a box of 32 x 64 dots. The coordinates of the dots comprising each character, i.e., C, Br, horizontal dash and vertical dash are stored as XXYY and unpacked to ØØXX and ØØYY. These coordinates are added to the origin setting, loaded into the x and y-axis DAC's and displayed.

Once all five carbons are entered, the voltages of the four Lab-8 knobs are read by the ADC and stored. They are packed into 2 single words and displayed using the same character display routine.

The heart of the entire program is the subroutine PSKLST, called by JMS I SKLTST, which tests whether the packed coordinate in the AC on entering is connected to any carbon so far entered. If it is connected in the y direction, the coordinates differ by ØØ1Ø. If it is connected in the x direction, the coordinates differ by 1ØØØ for carbons and 1ØØØ or Ø4ØØ for bromines. If any connections are found, the register CWORD contains bits set in the following manner for up, down, right, and left connections of the original coordinate to the carbon skeleton: UDØ ØØØ ØØØ ØRL.

In addition, the table CONECT contains words with bits set corresponding to which of the carbon skeleton words are connected. For example, if the coordinates in the AC are connected to the second carbon in the list, and that carbon lies below the coordinates in the AC, the second entry in the CONECT table will contain Ø1Ø ØØØ ØØØ ØØØ.

The logical flow of compound identification is based entirely on this routine and on the conventional rules for naming carbon compounds.

1. Find the Longest Chain

The first carbon in the input list is examined to see where it is connected, in the order R, L, U, D until a connection is formed. The connected carbon is then examined to see where it is connected, and so on. In each case a mask is ANDed with the connection word CWORD, to prevent backtracking in the direction which it just came from. When a carbon is reached which contains no new connections, i.e., the end of the chain, this chain length is put in NTEMP, and the coordinates of the chain in the TEMP table. The length of the TEMP table is compared with the PERM table and the TEMP table written into the PERM table if it is longer. Chain connection tests are then made on each of the remaining carbons so that the longest chain found is finally written into the PERM table and its length in NPERM.

2. Test for Chain Length

If the longest chain found is 2 or less, the error message NOT ENOUGH CARBONS is typed. If C is typed when five carbons are already displayed the error message TOO MANY CARBONS is typed and the whole entry erased.

If the longest chain found is 3, 4, or 5, and five carbons have been entered, jumps are performed to CHAIN3, CHAIN4 or CHAIN5.

3. CHAIN3

The PERM chain is written into the input list, with the two non-chain carbons last. If the second carbon of the chain is connected to four others a legal neopentyl structure is being displayed. If the two bromines are connected to the same carbon the name 1,1-dibromo-2, 2-dimethylpropane is typed. If they are connected to different carbons the indices are 1,3.

4. Checking off in the Table

When a legal structure is found, the table CnTABL is searched for a match. When it is found, bit Ø (the sign bit) is tested. If bit Ø is zero, the compound has not yet been done. Bit Ø is then set to 1 so that future tests will generate the message YOU HAVE ALREADY DONE. If the compound has not been done, the message THAT IS is typed, followed by the name of the compound.

5. CHAIN4

The PERM chain is written into the input list, with the one non-chain carbon (the branched C) at the end of the list. A test is made to see if the C-methyl carbon is connected to carbon 3. If connected to C-3, the order of the first four carbons is reversed so that the C-methyl carbon is connected to C-2.

The bromines are then tested and assigned indices according to the number of the carbon in the sorted list. If a bromine is connected to the C-methyl carbon and to C-1 the name 1-bromo-2-bromomethylbutane is typed. If a bromine is connected to the C-methyl carbon but not to C-1, C-1 and C-methyl are interchanged.

The indices of the bromines are then summed. If the sum is greater than five, each index is subtracted from five and the compound is named as an n,n-dibromo-3-methylbutane. If the sum is less than or equal to five, the compound is named as an n,n,-dibromo-2-methylbutane.

6. CHAIN5

The PERM chain is written into the input list, providing an order for the chain when the bromine indices are found. These indices are determined, and if their sum is greater than six they are subtracted from six to determine their actual value. This is equivalent to counting from the other end of the chain.

7. Done

When D is typed a search is made through the tables of indices of legal compounds C3TABL, C4TABL, and C5TABL for any numbers which are not negative. If any are found the message SORRY,...etc. is typed followed by the names of any compounds found. The SORRY message is disabled from typing after its first appearance. When the testing is done, bit Ø of all values in all tables is set to zero again and the program is restarted at the beginning.

8. Tables

```
C3TABL,   0011        C4TABL,   0011 /COMPOUNDS NAMED AS 2-METHYLBUTANES
          0013                  0012
                                0013
                                0014
                                0023

C5TABL,   0011        C3MTAB,   0011 /COMPOUNDS NAMED AS 3-METHYLBUTANES
          0012                  0012
          0013                  0013
          0014                  0022
          0015
          0022
          0023
          0024
          0033

CS,       1000 /DOTS COMPRISING C's
          2000
          3000
          0010
          0020
          0030
          0040
          1050
          2050
          3050
```

```
HDASH,    0020 /HORIZONTAL DASH
          1020
          2020
          3020

VDASH,    1020 /VERTICAL DASH
          1030
          1040
          1050
          1060

POIDOT,   1100 /POINTER
          1500
          2100
          2500
          1303
          1703
          2303
          1506
          2106
          1711

BR,       0010 /BROMINE
          0020
          0030
          0040
          0050
          1000
          1020
          1050
          2000
          2020
          2050
          3010
          3030
          3040
          5000
          5010
          5020
          5030
          6020
          7020
```

IDENTIFY ALL THE ISOMERS OF C5H10BR2
TYPE 'I' FOR COMPLETE INSTRUCTIONS

TO USE THIS PROGRAM:

CONSTRUCT CARBON CHAINS BY TYPING C'S
A 'C' WILL APPEAR ON THE SCOPE AT THE POINTER
TO MOVE THE POINTER, TYPE:
    SPACE - TO MOVE IT TO THE RIGHT
    RETURN - TO MOVE TO START OF NEXT LINE
    LINE FEED - TO MOVE STRAIGHT DOWN
    <— TO BACK UP ONE SPACE
    ↑ TO MOVE UP ONE LINE
    RUBOUT - TO ERASE THE LAST CARBON TYPED
DASHES WILL APPEAR BETWEEN CONNECTED CARBONS

WHEN YOU HAVE TYPED 5 CARBONS, 2 BR'S WILL APPEAR ON THE SCOPE
THEIR POSITIONS ARE ADJUSTED BY THE 4 KNOBS ON THE LAB-8
KNOBS 0 AND 1 CONTROL THE X AND Y COORDINATES OF ONE BR
AND KNOBS 2 AND 3 THE COORDS OF THE OTHER

WHEN YOU HAVE ADJUSTED THE STRUCTURE, TYPE:
N- TO ENTER THE NAME IN THE LIST OF COMPLETED COMPOUNDS
    I WILL TYPE OUT THE NAME OF EACH ISOMER AS YOU ENTER IT
    AFTER EACH N, MOVE THE BR'S WITH THE KNOBS AND TYPE N AGAIN OR TYPE:
CONTROL/E - TO ERASE THE ENTIRE STRUCTURE
D- WHEN YOU THINK YOU HAVE ENTERED ALL THE ISOMERS
I- TO TYPE OUT THIS LIST OF INSTRUCTIONS
CONTROL/R- TO START NAMING COMPOUNDS ALL OVER AGAIN
DO NOT TYPE CONTROL/C UNLESS PS-8 OR DISK MONITOR IS RESIDENT
GOOD LUCK!!

THAT IS 1,1-DIBROMOPENTANE
THAT IS 1,2-DIBROMOPENTANE
THAT IS 1,3-DIBROMOPENTANE
THAT IS 1,4-DIBROMOPENTANE
THAT IS 1,5-DIBROMOPENTANE
THAT IS 2,2-DIBROMOPENTANE
THAT IS 2,3-DIBROMOPENTANE
THAT IS 2,4-DIBROMOPENTANE
THAT IS 3,3-DIBROMOPENTANE
THAT IS 1-BROMO-2-BROMOMETHYLBUTANE
THAT IS 1,1-DIBROMO-2-METHYLBUTANE
THAT IS 1,2-DIBROMO-2-METHYLBUTANE
THAT IS 1,3-DIBROMO-2-METHYLBUTANE
THAT IS 1,4-DIBROMO-2-METHYLBUTANE
THAT IS 2,3-DIBROMO-2-METHYLBUTANE
THAT IS 1,3-DIBROMO-3-METHYLBUTANE

THAT IS 2,2-DIBROMO-3-METHYLBUTANE
THAT IS 1,2-DIBROMO-3-METHYLBUTANE
THAT IS 1,1-DIBROMO-3-METHYLBUTANE
THAT IS 1,3-DIBROMO-2,2-DIMETHYLPROPANE
THAT IS 1,1-DIBROMO-2,2-DIMETHYLPROPANE

EXCELLENT! YOU FOUND ALL 21 ISOMERS
PLEASE SEND IN THE NEXT STUDENT

IDENTIFY ALL THE ISOMERS OF C5H10BR2
TYPE 'I' FOR COMPLETE INSTRUCTIONS