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A MICROCOMPUTER SIMULATION OF THE INVERSION VIBRATION OF THE AMMONIA MOLECULE

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ABSTRACT

An algorithm is presented for computing the bond angles in ammonia in terms of the inversion energy barrier. This algorithm has been implemented on a microcomputer and its accompanying graphics printer to show perspective structures of the inverting molecule at various bond angles. A complete program listing and user instructions are presented.

INTRODUCTION

An enormously powerful and versatile generation of microcomputers is available for teaching and research purposes. These machines include "pocket" computers with impressive computational and graphics capability. In the course of carrying out computations of molecular structure and conformation, it became desirable to relate the energy of pyramidal (C_{3v}) molecules to the actual configuration as inversion occurs and to show these configurations graphically. A pocket computer has been used for this work and we present here the details of the algorithm and the implementation of the program in BASIC.

PRINCIPLES

The representation of a molecular potential energy function as a parabola is well known (King, 1964). In the case of the inversion vibration (ν_2) of pyramidal molecules like NH_3, there is a barrier to the inversion which is related to the bond angle. For NH_3, the inversion barrier is 2020 cm $^{-1}$ (Hollas, 1982) and the normal bond angle, HNH, is 107.3° (DeKock and Gray, 1980). Therefore, when the bond angle is 120° (planar D_{3h} structure where the angle expansion is 12.7°) the energy of the configuration is 2020 cm^{-1}. The potential energy curve is shown in Figure 1. For the present computation, we have assumed that the potential energy for compression of the bond angle by 12.7° would also require an energy of 2020 cm^{-1} so

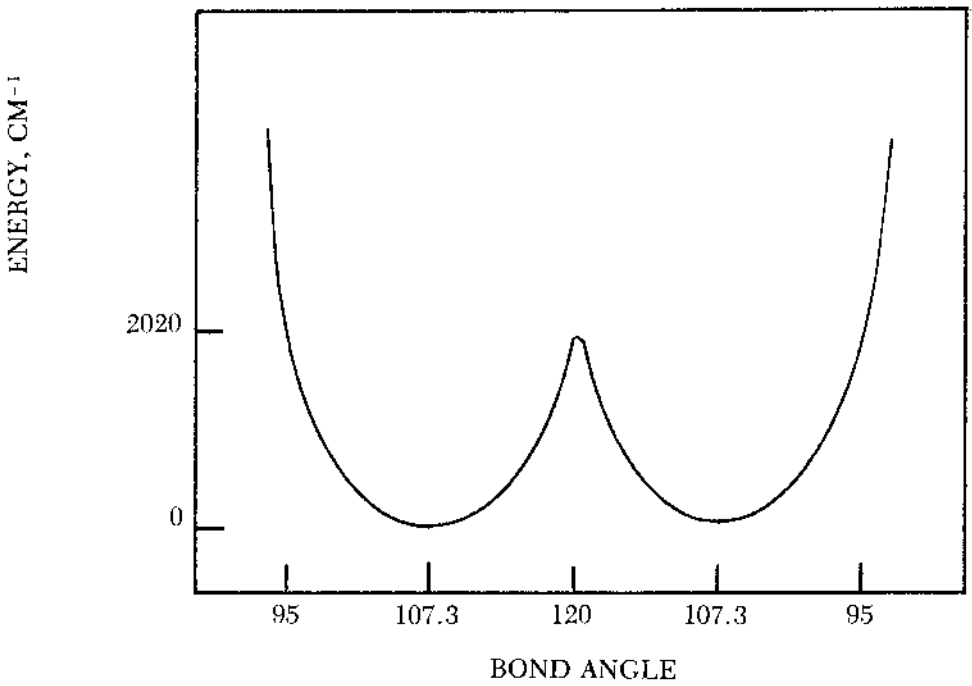

Fig. 1. Potential energy curve for the inversion of NH_3.

that each potential well is symmetrical with respect to increase or decrease of the HNH bond angle. Thus, the energy is assumed to be 2020 cm $^{-1}$ at bond angles of 120 and 95 and to be 0 cm $^{-1}$ at 107.3. Using the energies at these three bond angles, the parabolic relationship between energy and bond angle was established in order to calculate the energy at intermediate bond angles. A pocket computer programmed in BASIC was used to compute the energy and to draw the molecule at the desired bond angles.

ALGORITHM

Computation of the conformational energy of NH_3 at several bond angles was carried out and the graphical representation of each structure was drawn using a Radio Shack PC-2 pocket computer with a graphics plotter. At each bond angle, the x, y, and z-coordinates of each atom are calculated. Then, the horizontal and vertical angles between these coordinates and a fixed "eye" point and a "focus" point are calculated. These angles are then projected through a plane to yield a series of (x,y) points which are then plotted by the plotter. After the NH_3 molecule is drawn, the energy of the molecule at that bond angle is calculated using the parabolic approximation as the potential function. Finally, the HNH bond angle is incremented (or decremented) depending on the current motion and the process continues until the completed cycle of the vibration is complete. In running the program, the normal bond angle (NA) and the barrier energy (BE) are included in lines 100 and 110. These parameters may be changed at the user's discretion thus making the program adaptable to other pyramidal molecules. Also, the bond angle increment (BI) is specified in line 120. The starting value for the current bond angle (BA) is specified in line 130. A complete listing of the program in BASIC and a data dictionary are shown in the Appendix.

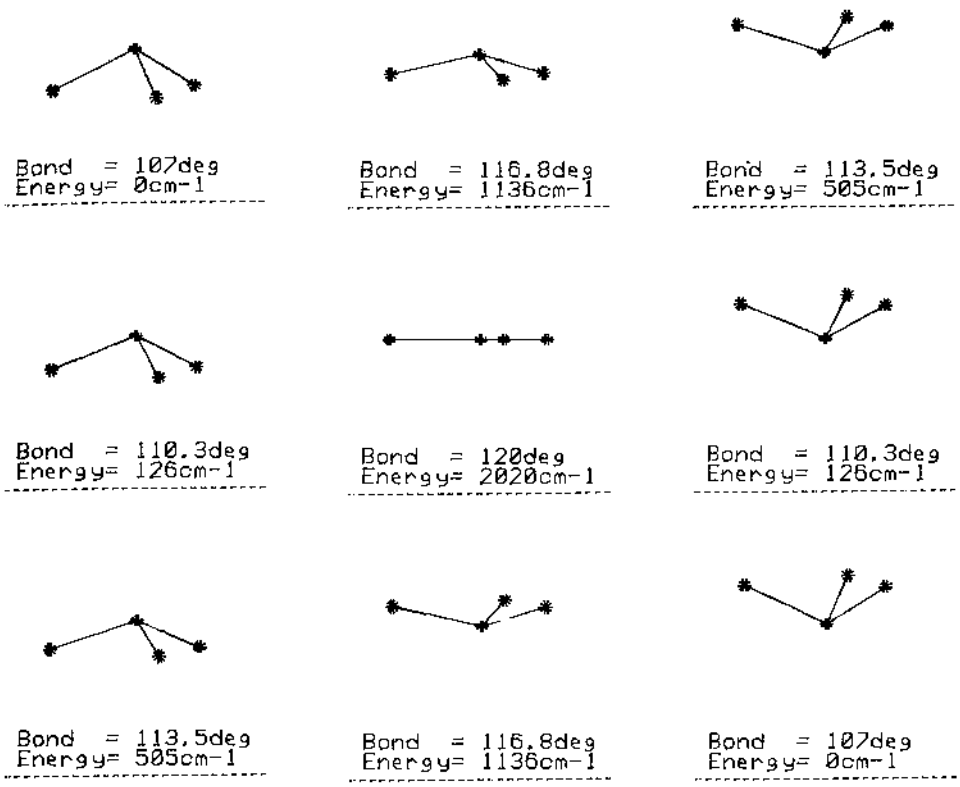

Fig. 2. Stages in a complete vibration of NH_3.

RESULTS AND DISCUSSION

Application of the program to the simulation of the inversion vibration of NH_3 produces the series of diagrams shown in Figure 2. The number of drawings produced to show a complete vibration can be varied by the program user. Therefore, in creating a motion effect, the number of drawings could be quite large with small changes in bond angle between each drawing. It is clear that the graphics capability of the pocket computer enables it to be a useful tool in showing molecular vibrations when suitable software is available. Certainly the production of perspective drawings, not just images on a display, showing the details of a molecular vibration in a "stop action" mode is of considerable heuristic value. We are currently developing other programs for using microcomputers to obtain a variety of molecular parameters and to show energy and structure relationships for both teaching and research applications.

LITERATURE CITED

DeKock, R.L. and Gray, H.B. 1980. Chemical Structure and Bonding. Benjamin/Cummings Publishing Co., Menlo Park, CA.

Hollas, J.M. 1982. High Resolution Spectroscopy. Butterworths, London, pp. 252-256.

King, G.W. 1964. Spectroscopy and Molecular Structure. Holt, Rinehart, and Winston, New York, pp. 357-360.

APPENDIX

PROGRAM DATA DICTIONARY

Name (DIM)	Description	Name (DIM)	Description
A	Atom ray angle	LL	Bond length
A (NP,1)	Atom horiz. angle	LT (NP)	Line type array
A (NP,2)	Atom vert. angle	L1	Loop counter 1
BA	H-N-H bond angle	L2	Loop counter 2
BE	Barrier energy	NA	Normal angle
BI	Angle increment	NP	No. XYZ pts.
DF	Dist. to focus pt.	P (NP,3)	Atom XYZ coord.
EX	Eye X coord.	PD	Dist. to plane
EY	Eye Y coord.	PW	Width of plane
EZ	Eye Z coord.	PX	Plotter X coord.
FX	Focus X coord.	PY	Plotter Y coord.
FY	Focus Y coord.	TA	Temporary angle
FZ	Focus Z coord.	VA	Vert. focus ang.
HA	Horiz. focus angle	VM	Vector magnifier
LA	Leg angle		

PROGRAM LISTING

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10Ø:NA=1Ø7
11Ø:BE=2Ø2Ø
12Ø:BI=3.25
13Ø:BA=1Ø7
14Ø:DEGREE :GRAPH
    :GLCURSOR (1Ø8
    ,1Ø8):SORGN :
    CSIZE 2
15Ø:DIM P(99,3),A(
    99,2),LT(99):N
    P=1Ø
16Ø:EX=1:EY=1:EZ=2
   :PD=1:PW=.5:VM
    =216/PW:LL=1:N
    P=6
17Ø:LINE (-1Ø7,1Ø8
    )-(1Ø8,1Ø8),3,
    Ø
18Ø:FX=5:FY=5:FZ=2
19Ø:IF BA=16ØLET B
    I=BI*-1
2ØØ:IF BA=8ØLET BI
    =BI*-1
21Ø:TA=BA:IF BA>12
    ØLET TA=24Ø-BA
22Ø:LA=ASN (TA/12Ø
    ):IF BA>12ØLET
    LA=18Ø-LA
23Ø:P(1,1)=FX:P(1,
    2)=FY:P(1,3)=F
    Z:LT(1)=9
24Ø:P(2,1)=FX+SIN
    LA*COS Ø*LL:P(
    2,2)=FY+SIN LA
    *SIN Ø*LL:P(2,
    3)=FZ-COS LA*L
    L:LT(2)=Ø
25Ø:P(3,1)=FZ:P(3,
    2)=FY:P(3,3)=F
    Z:LT(3)=9
26Ø:P(4,1)=FX+SIN
    LA*COS 12Ø*LL:
    P(4,2)=FY+SIN
    LA*SIN 12Ø*LL:
    P(4,3)=FZ-COS
    LA*LL:LT(4)=Ø
27Ø:P(5,1)=FX:P(5,
    2)=FY:P(5,3)=F
    Z:LT(5)=9
28Ø:P(6,1)=FX+SIN
    LA*COS 24Ø*LL:
    P(6,2)=FY+SIN
    LA*SIN 24Ø*LL:
    P(6,3)=FZ-COS
    LA*LL:LT(6)=Ø
29Ø:FX=FX-EX:FY=FY
    -EY:FZ=FZ-EZ
3ØØ:FOR L1=1TO NP
31Ø:P(L1,1)=P(L1,1
    )-EX
32Ø:P(L1,2)=P(L1,2
    )-EY
33Ø:P(L1,3)=P(L1,3
    )-EZ
34Ø:NEXT L1
35Ø:VA=ATN (FZ/SQR
    (FX^2+FY^2))
36Ø:HA=ATN (FY/FX)
37Ø:DF=SQR (FX^2+F
    Y^2+FZ^2)
38Ø:FOR L1=1TO NP
39Ø:A(L1,1)=ATN (P
    (L1,3)/SQR (P(
    L1,1)^2+P(L1,2
    )^2))-VA
4ØØ:A(L1,2)=ATN (P
    (L1,2)/P(L1,1)
    )-HA
41Ø:A(L1,2)=ATN (
    TAN A(L1,2)/(D
    F/SQR (P(L1,1)
    ^2+P(L1,2)^2))
    )
42Ø:NEXT L1
43Ø:FOR L1=1TO NP
44Ø:PY=+PD*TAN (A(
    L1,1))*VM
45Ø:PX=-PD*TAN (A(
    L1,2))*VM
46Ø:LINE -(PX,PY),
    LT(L1)
47Ø:IF L1=3OR L1=5
    THEN Ø52Ø
48Ø:FOR L2=1TO 1Ø
49Ø:A=36*L2
5ØØ:LINE (PX+COS A
    *5,PY+SIN A*5)
    -(PX,PY),Ø
51Ø:NEXT L2
52Ø:NEXT L1
53Ø:GLCURSOR (-1Ø8
    ,-1ØØ)
54Ø:TA=BA:IF BA>12
    ØLET TA=24Ø-BA
55Ø:LPRINT "Bond
     =";INT (TA*1Ø
    +.5)/1Ø;"deg"
56Ø:GLCURSOR (-1Ø8
    ,-116):LPRINT
    " Energy=";INT
    ((BE/(12Ø-NA)^
    2)*(TA-NA)^2+.
    5);"cm-1"
57Ø:GLCURSOR (Ø,-2
    32):SORGN
58Ø:BA=BA+BI
59Ø:GOTO 17Ø
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