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IMPLEMENTATION OF TWO PROGRAMS IN PC-COMPUTER

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ABSTRACT

Two programs were installed in PC-Computer one of which is concerned with the geometry of the molecules, namely, the program XANDU, the other one is a program for solving crystal structures using direct methods and Paterson techniques (SHELX86). The accuracy of the data obtained were compared with those taken from the main fraim computers and were found to be in good agreement.

Requirements for Installation:

The program XANDU (Roberets & Sheldrik) and the Pc version of SHELX86 written by Sheldrik (1986) were installed in the Pc-computer with Intel 80286 processor, an 80287/6 numeric coprocessor, 20 MB main memory and 1.2 RAM disk. The operating system of the PC-computer is PC-DOS version 2.1 . In the program XANDU 1600 statement (FORTRAN-77) were fed into the computer through the keyboard and some modifications were made to the original version.

Program XANDU :

This program provides a variety of crystallographic

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calculations for all space groups such as:

1- Calculations of bond lengths and bond angles.
2- Torsion angles.
3- Best least square planes through atoms.
4- Libration analysis of possible rigid molecule motion.

In order to test the program, the structure of 8-aza guanine hydrobromide monohydrate Kozlowsk, 1975) was undertaken. The chemical formula of the copound is $C_4H_7N_6Br$, then numbering scheme is shown in figure (1). This compound crystalizes in the monoclinic system and has a space group $P2_1/n$. The unit cell diamensions are: a=5.809(3), b=13.073(8), c=10.899(7) A°, β=84.45(2) and Z=4.

Fractional coordinates, listed in table (1) were taken from which bond lengths and bond angles were calculated in the PC-computer. It was found that the difference between the values calculated in the main frame and those in PC-computer occur only in the third decimal, table (2) and (3). Further calculations of the torsion angles and best least square planes through atoms were carried out, tables (4) and (5). These show that the five membered triazole ring and the pyrimidine ring (N1, C2, N3, C4, C5 and C6) are planar within experimental errors. The dihedral angle between the two rings was 0.92°, which indicates that there is slight pucker along C4-C5.

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Programe SHELX-86:

SHELX-86 is a fortran 77 programe for the solution of crystal structure from X-ray diffraction data. This programe suitable for structures up to 200 atoms in the asymmetric unit, is efficient for all space group in all settings and there is no linit on the number of reflections.

The first test job was for location of the heavy atoms from an E-map, using the Patterson technique. A structure of 144 C, 264 H, 8 N, 24 S, 8 Cu and 4 Mo in the unit cell which crystalises in the space group C2/c was undertaken The diffraction data were collected using Mo K_α ($\lambda = 0.71069$ Å) and the unit cell was found to be : a= 17.064, b= 15.646, c = 18.448 A° and β= 110.47°. 4059 reflections were collected from which 3059 reflections were unique. Patterson synthesis was carried out and the heavy atoms were located, table (6). The time for that job was 20 minutes. The second test job was for solving the structure using direct methods technique. A crystal of 68 C, 104 H, 40 O atom per unit cell was undertaken. The compound crystalises in space group $P2_12_12_1$ and has cell dimensions of a=8.187, b=14.277 and c=15.693 A. 2428 unique reflections were collected using MoK_α (λ =.71069) from which 2177 reflctions were observed ($I > 5\sigma$). The observed structure factors (F) were converted to their corresponding point atoms (E) and 20 phase sets were calculated, the one having the best figure of merit was chosen. This solution

was extended by tangent expansion and then an E-map was calculated. The point atom relaibility factor based on 694 E-values was Re=0.184. The line printer plot of the structur at this stage was interpreted with the aid of bond lengths and bond angles calculated by the programe. The drawing obtained for this trial structer is shown in figure (2).

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Table (1)

Fractional coordinates for the nonhydrogen atoms.

Atom	X	Y	Z
O6	0.1085(7)	0.1979(3)	0.3249(3)
N1	0.0247(9)	0.3671(3)	0.3322(4)
N2	-0.4156(10)	0.0351(4)	0.1438(5)
N3	0.2578(8)	0.4959(3)	0.2376(4)
N7	-0.4589(9)	0.2642(3)	0.1594(4)
N8	-0.3241(10)	0.3351(4)	0.1054(5)
N9	-0.3962(8)	0.4323(3)	0.1224(4)
C2	0.0666(9)	0.4682(4)	0.2295(5)
C4	0.4020(9)	0.4208(4)	0.1927(5)
C5	0.3634(9)	0.3184(4)	0.2163(4)
C6	0.1652(9)	0.2840(4)	0.2936(4)

Table(2)

Bond lengths (Å).

Atom1--Atom2	Main Frame	PC-Computer
N1-----C2	1.365	1.364
C2----N3	1.339	1.340
N3----C4	1.352	1.351
C4----C5	1.377	1.377
C5----C6	1.432	1.432
C6----N1	1.398	1.399
C5----N7	1.353	1.352
N7----N8	1.315	1.315
N8----N9	1.345	1.345
N9----C4	1.345	1.345
C2----N2	1.310	1.311
C6----O6	1.212	1.212

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Table (3)

Selected bond angles (°).

Atom1--Atom2--Atom3	Main Frame angle	PC-Computer angle
C6-----N1-----C2	127.4	127.4
N1-----C2-----N3	119.6	119.6
N1-----C2-----N2	118.1	118.1
N2-----C2-----N3	122.3	122.3
C2-----N3-----C4	117.6	117.6
N3-----C4-----C5	128.7	128.7
N9-----C4-----C5	109.4	109.4
N3-----C4-----N9	126.9	126.9
C4-----C5-----C6	121.5	121.5
N7-----C5-----C6	129.8	129.8
C4-----C5-----N7	108.7	108.7
C5-----C6-----N1	110.2	110.2
C5-----C6-----O6	129.6	129.7
N1-----C6-----O6	120.1	120.1
C5-----N7-----N8	103.3	103.4
N7-----N8-----N9	116.1	116.1
C4-----N9-----N9	102.5	102.4

Table(4)

Selected Torsion angle (°) ,calculated by PC-Computer.

Atom1-Atom2-Atom3-Atom4	Angle
C6-----N1-----C2-----N3	2.24
C2-----N1-----C6-----C5	-3.35
C4-----N3-----C2-----N1	0.00
C2-----N3-----C4-----C5	0.00
C5-----N7-----N8-----N9	0.00
N8-----N7-----C5-----C4	0.00
N7-----N8-----N9-----C4	-0.91
N8-----N9-----C4-----N3	180.0
N8-----N9-----C4-----C5	0.89
N3-----C4-----C5-----C6	-1.14
N9-----C4-----C5-----N7	0.00
N7-----C5-----C6-----O6	-1.11
C4-----C5-----C6-----N1	2.68

Table (5)

Deviation of atoms from mean plane

Plane No.	Atom	Deviation from plane
1	N1	-0.0100
	C2	0.0023
	N3	0.0067
	C4	-0.0021
	C5	-0.0095
	C6	0.0126
2	N7	0.0139
	N8	-0.0021
	N9	0.0057
	C4	-0.0043
	C5	0.0022

Table (6)

The positons of the heavy atoms

Atom	X	Y	Z
Mo	0.000	0.061	0.250
Cu	-0.155	0.061	0.157
S	0.100	0.142	0.240
S	-0.057	-0.021	0.148
S	-0.304	0.063	0.072

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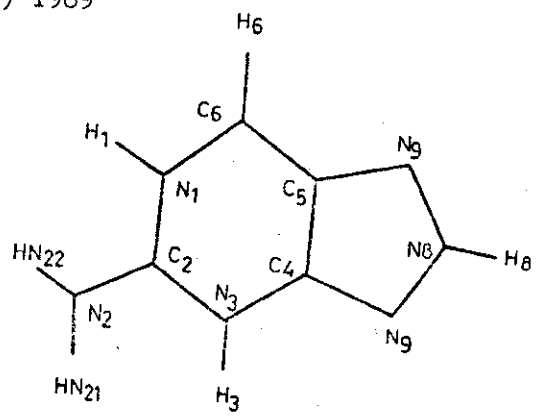

Figure (1)

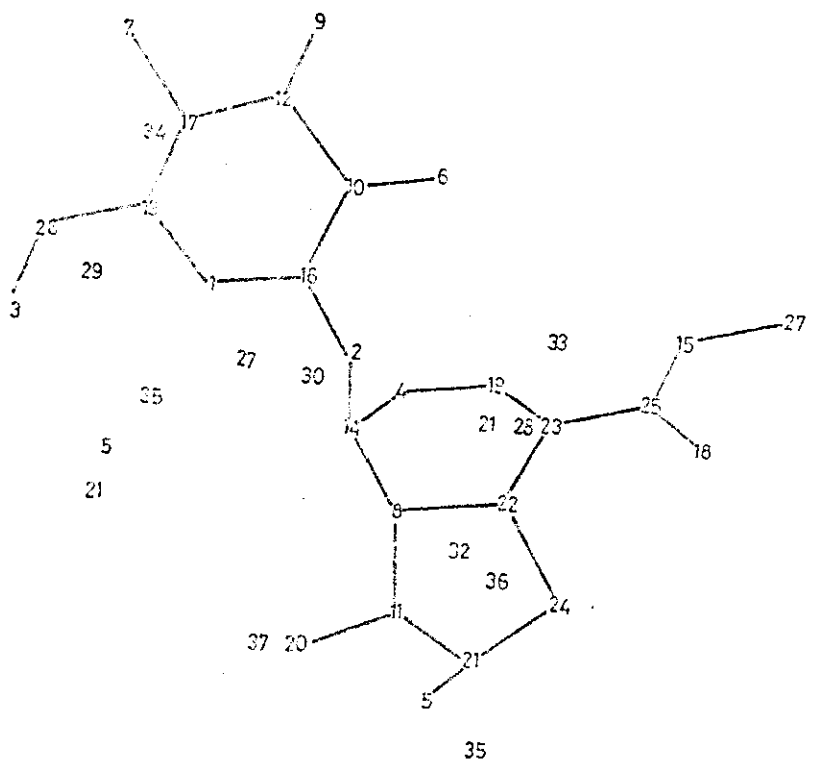

Figure (2)

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تخزين بعض البرامج وتنفيذها من خلال الكمبيوتر الشخصى

عبد الفتاح ابراهيم الشورة
قسم الطبيعة ـ كلية العلوم جامعة طنطا

تم تخزين برنامجين داخل الكمبيوتر الشخصى ، البرنامج الاول وهو خاص بالحسابات الهندسية للجزئ والاخر يتصل بحل المركب اما باستخدام الطريقة المباشرة أو باستخدام طريقة الباترسون فى الابعاد الثلاثة. قورنت النتائج المتاحة من الكمبيوتر الشخصى وتلك التى اخذت من الحاسب الالى ووجد أن النتائج تقريبا متطابقة.