

The Crystal and Molecular Structure of Chlorpropamide

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Abstract—Chlorpropamide, $C_{10}H_{13}N_2O_3$ SCl, forms orthorhombic crystals of space group $P_{2,2,2}$, with a 9.066 ± 0.004 , $b = 5.218 \pm 0.003$, $c = 26.604 \pm 0.008$ Å, and four molecules per cell. Three dimensional photographic data were collected with Mo-K α radiation. The structure was determined using Patterson, Fourier and Difference syntheses methods and refined by the block-diagonal least-squares methods with anisotropic thermal parameters for all nonhydrogen atoms and isotropic thermal parameters for all hydrogen atoms. The final R value was 0.10 for the 1823 observed independent reflections. The dihedral angle between the planes through the benzene ring and the urea group is 99° . The conformational angle formed by the projection of the S-C(1) with that of N(1)-C(7) when the projection is taken along the S-N(1) bond is 76° . The molecule appears to form with neighbouring molecules two hydrogen bonds, N(1)-H...O(3) and N(2)-H...O(2) of lengths 2.774 and 2.954 Å respectively related by screw diads parallel to the a axis. Adjacent molecules parallel to b and c axis are bound together by van der Waals forces.

Keywords—Chlorpropamide—crystal and molecular structure. X-ray diffraction method—Patterson, Fourier and difference syntheses methods—block-diagonal least-squares methods.

To solve the relationship between the stereochemical structure of a molecule and its biological action is one of the important contributing factors for the development of molecular biology or molecular pharmacology.

Some of the concerned examples are as

follows: 1). On neurochemical transmitters: It has been found that a) acetylcholine and ω -aminoacids of this sort act as the chemical transmitters inhibiting the peripheral nervous system and b) glycine, β -alanine and γ -amino-butylic acid seem to act as chemical transmitters inhibiting central nervous system in mammals.

We have number of research papers^{1~8)} which deal with the relationship between chemical structures and biochemical activities taking into consideration of their stereochemical structures found by the structure-analysis of these compounds. It is noted that Beers and Reich³⁾ studied the structures of receptors for donors, the above mentioned chemical transmitters. 2). On anti-cancer compounds: among α -(N)-heterocyclic thiosemicarbazone derivatives, there have been found a lot of anti-cancer compounds. It was assumed that these compounds should form octahedral tridentate chelate complex with metallic ions in order to have the anti-cancer activities. So, the studies of stereochemical structure analysis have been undertaken^{9~12)}. 3). On anti-bacterials compounds: a number of sulfonyl-group containing compounds are found to have antibacterial activities. Molecular structures of these compounds, in details, have been studied^{13~22)}

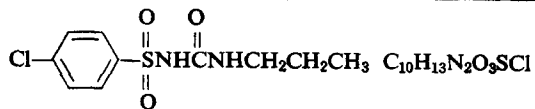
Stereo-chemical structure of the above mentioned biologically active compounds ought to be studied to obtain conclusive relationships between biological activities and molecular structures. In addition to these studies, molecular biological studies must be also undertaken for finding out the structures of the concerned receptors. It has been found that anti-diabetics lower the blood-sugar level by stimulating β -cells of Langerhans' island of the pancreas.

For the purpose of finding out a relationship between the stereo-chemical structures of antidiabetics and their biological activities, a strong antidiabetic, chlorpropamide, which contains both sulfonyl and urea groups, was studied for its stereo-chemical structure, lengths and angles of bonds, conformation angles and hydrogen bonding schemes, by using X-ray diffraction methods.

EXPERIMENTAL

Crystals of chlorpropamide were obtained from ethanol solution by slow evaporation at room temperature. They were colourless and needle in shape. The unit-cell dimensions were determined from the Weissenberg photographs about the two principal axes taken with Mo-K α radiation and refined by the least-squares method with the spacings of ten Okl and twelve hOl reflections at high angles, calculated with those of the superimposed Al powder lines. The observed density measured by floatation in solutions of carbontetrachloride and benzene. The crystal data are given in Table I.

Table I: The crystal data of Chlorpropamide



M. W. = 276.5

Unit cell parameters : $a=9.066(4)$ Å, $b=5.218(3)$,
 $c=26.604(8)$, $Z=4$, $V=1258.54$ Å³

Space group : $P_{2,2,2}$

from systematic absences, hOO : $h=2n+1$,

OkO : $k=2n+1$, OOl : $l=2n+1$

Density : calculated value 1.46 gcm,
measured value 1.47

The X-ray reflection data were estimated visually from sets of multiple-film equi-inclination Weissenberg photographs taken at room temperature about the a -(2 layers, Okl to 1kl) and b -(7 layers, hOl to h6l) axes, with Zr-filtered Mo K α radiation, using two crystals. The approximate dimensions of the crystals were $0.2 \times 0.2 \times 0.1$ mm. In this way the intensities of 1823 independent reflections were measured and used in the crystal analysis. Corrections for Lorentz and polarization effects were made in the usual way. No corrections for absorption and extinction were made. An absolute scale factor and mean isotropic temperature factor were obtained by Wilson's method and normalized structure factor, E , were calculated. All calculations were performed on the IBM 360 computer, using the programs written by Shiono²³).

STRUCTURE DETERMINATION AND REFINEMENT

The coordinates of the chlorine and sulfur atoms were deduced from a three dimensional

Patterson function. A Fourier synthesis based on the coordinates of the two atoms revealed positions of all the non-hydrogen atoms. The refinement was carried out by the block-diagonal least-squares method, at first with isotropic, then with anisotropic thermal parameters, resulting in a discrepancy index R of 0.13. A three-dimensional difference

Fourier synthesis was calculated at this stage and all the hydrogen atoms were located. Least-squares refinement was then made having assigned isotropic temperature factors to the hydrogen atoms. The weighting scheme proposed by Cruickshank²⁴⁾ was used. The final R value is 0.10 for the 1823 reflections. The atomic coordinates and thermal

Table II: Fractional atomic coordinates and anisotropic thermal parameters in chlorpropamide.

	X	Y	Z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cl	0.2786(4)	0.2168(7)	0.2595(1)	0.0313(6)	0.076(2)	0.00194(5)	-0.0017(9)	-0.0005(1)	-0.0042(2)
S	0.2244(2)	-0.5261(2)	0.0775(1)	0.0107(2)	0.031(1)	0.00125(2)	0.0004(3)	0.0019(5)	0.0007(1)
C(1)	0.2407(6)	-0.317(1)	0.1290(2)	0.0124(7)	0.039(2)	0.0015(1)	0.002(1)	-0.0001(2)	0.0008(3)
C(2)	0.1277(9)	-0.307(2)	0.1643(3)	0.016(1)	0.066(4)	0.0016(1)	-0.005(2)	0.0003(3)	0.0004(6)
C(3)	0.1421(9)	-0.145(2)	0.2049(3)	0.019(1)	0.072(5)	0.0018(1)	0.000(2)	0.0011(3)	-0.0017(6)
C(4)	0.2650(9)	0.009(2)	0.2091(3)	0.021(1)	0.054(3)	0.0016(1)	0.001(2)	-0.0009(3)	-0.0002(5)
C(5)	0.3761(9)	0.003(2)	0.1742(3)	0.017(1)	0.048(3)	0.0020(2)	-0.003(2)	-0.0003(3)	0.0002(6)
C(6)	0.3629(8)	-0.158(2)	0.1339(3)	0.014(1)	0.050(3)	0.0018(1)	-0.002(2)	0.0007(3)	0.0008(5)
C(7)	0.2427(7)	-0.179(1)	0.0028(3)	0.013(1)	0.045(3)	0.0015(1)	-0.001(1)	0.0000(2)	0.0004(4)
C(8)	0.2199(8)	0.173(2)	-0.0578(3)	0.015(1)	0.043(3)	0.0017(1)	0.001(2)	0.0002(3)	-0.0003(4)
C(9)	0.2350(9)	0.103(2)	-0.1121(3)	0.019(1)	0.056(4)	0.0017(1)	-0.001(2)	0.0002(3)	-0.0007(5)
C(10)	0.2855(9)	0.332(2)	-0.1418(4)	0.018(1)	0.074(5)	0.0022(2)	0.006(2)	-0.0013(3)	-0.0042(7)
O(1)	0.1092(7)	-0.703(1)	0.0877(2)	0.020(1)	0.053(2)	0.0025(1)	-0.004(1)	0.0003(2)	0.0017(4)
O(2)	0.3676(6)	-0.617(1)	0.0656(2)	0.018(1)	0.047(2)	0.0021(1)	0.005(1)	0.0004(2)	0.0007(3)
O(3)	0.3765(6)	-0.165(1)	0.0071(2)	0.160(7)	0.063(3)	0.0025(1)	0.000(1)	-0.0003(2)	-0.0019(4)
N(1)	0.1615(6)	-0.352(1)	0.0308(2)	0.012(1)	0.055(3)	0.0017(1)	-0.001(1)	-0.0003(2)	0.0010(4)
N(2)	0.1597(7)	-0.037(1)	-0.0267(2)	0.016(1)	0.060(3)	0.0021(1)	-0.000(1)	-0.0003(2)	-0.0024(5)
H1	0.037(5)	-0.420(9)	0.163(2)	5.8	} Isotropic temperature factors				
H2	0.040(5)	-0.150(9)	0.231(2)	6.6					
H3	0.469(5)	0.110(9)	0.186(2)	6.3					
H4	0.438(5)	-0.178(9)	0.102(2)	6.9					
H5	0.064(5)	-0.364(9)	0.025(2)	6.8					
H6	0.054(5)	-0.057(9)	-0.035(2)	6.0					
H7	0.156(5)	-0.700(9)	-0.054(2)	5.9					
H8	0.303(5)	-0.764(9)	-0.043(2)	5.5					
H9	0.288(5)	-0.936(9)	-0.091(2)	6.8					
H10	0.156(5)	-0.979(9)	-0.126(2)	6.3					
H11	0.296(5)	-0.720(9)	-0.174(2)	6.7					
H12	0.234(5)	-0.520(9)	-0.134(2)	6.6					
H13	0.379(6)	-0.666(9)	-0.143(2)	7.8					

Key to the atomic numbering is given in Fig. 1. The temperature factor expression used was $\exp[-(h^2\beta_{11} + K^2\beta_{22} + l^2\beta_{33} + 2hk\beta_{12} + 2hl\beta_{13} + 2kl\beta_{23})]$.

The estimated standard deviations in parentheses refer to the last decimal positions of the corresponding parameters.)

Table III: Observed and calculated structure factors for chlorpropamide.
 Columns are ; Index, Aobs, Acalc, Bobs, Bcalc.

h	k	l	h=0	l=0	h=3	l=1	h=4	l=2	h=6	l=3										
2	-41.01	-39.36	0.00	0.00	0	0	-0.00	-0.00	13.55	11.65	0	-47.92	-42.22	0.00	0.00	0	0.00	0.00	25.42	27.03
4	12.03	12.93	-0.00	-0.00	1	1	12.83	11.60	22.56	20.39	1	15.29	15.28	-36.85	-36.83	1	26.96	26.71	-12.91	-14.77
6	21.23	22.43	-0.00	-0.00	2	2	34.39	32.78	4.51	4.30	2	27.36	27.01	-5.17	-5.17	2	-16.48	-16.38	17.36	17.38
1	0.00	0.00	23.81	16.57	3	3	-5.90	-6.29	-8.39	-8.93	3	-8.58	-8.42	-16.49	-15.45	3	17.36	17.38	-2.02	-2.05
2	0.00	0.00	41.06	33.79	4	4	-18.20	-19.42	1.80	1.92	4	3.98	6.16	-9.49	-10.24	4	-5.18	-5.19	-5.03	-5.04
3	0.00	0.00	-22.89	-21.49	5	5	11.12	11.15	9.37	9.39	5	5.46	5.79	-8.24	-8.70	5	1.16	0.93	-2.84	-2.35
4	-0.00	-0.00	-9.58	-10.93	6	6	-8.00	-7.46	-0.93	-0.86	6	3.93	3.83	-4.25	-4.15	6	-4.61	-4.65	0.83	0.83
5	0.00	0.00	-2.33	-2.67	7	7	1.27	1.29	2.17	2.20	7	21.88	21.74	0.00	0.00	0	-0.00	-0.00	-44.42	-50.76
6	-0.00	-0.00	-8.53	-7.86	8	8	-0.00	-0.00	-60.38	-54.17	8	5.96	5.56	-12.84	-11.97	1	5.85	6.91	1.65	1.25
1	37.18	31.85	-0.00	-0.00	1	1	-30.05	-30.12	17.77	17.82	2	-29.01	-28.70	-4.58	-4.54	2	-15.74	-17.77	-14.81	-16.72
2	20.24	19.99	-0.00	-0.00	2	2	-25.24	-24.93	-26.99	-26.66	3	-10.49	-11.56	-27.43	-30.23	3	7.54	7.92	-3.04	3.08
3	-22.30	-24.42	0.00	0.00	3	3	2.40	2.65	20.43	22.40	4	-18.99	-19.86	-11.44	-11.96	4	8.51	8.44	-9.31	-9.45
4	-2.78	-2.75	-0.00	-0.00	4	4	17.50	18.25	-7.00	-7.30	5	8.12	-8.26	-2.39	-2.39	5	-0.20	-0.19	-3.67	-3.59
5	-13.04	-13.80	0.00	0.00	5	5	-5.90	-6.77	4.83	5.55	6	-2.66	-2.66	-1.33	-1.36	6	-0.00	-0.00	2.98	3.67
6	-3.03	-3.97	0.00	0.00	6	6	1.69	1.80	-4.47	-4.78	7	6.98	6.84	-0.00	-0.00	7	-17.55	-17.76	2.76	2.79
1	-0.00	-0.00	26.12	23.16	0	0	0.00	0.00	-10.05	-9.30	1	-5.59	-6.47	16.01	18.53	2	10.51	10.59	0.61	0.62
2	-0.00	-0.00	-42.85	-39.97	1	1	-7.56	-7.00	-17.24	-15.96	2	1.30	1.48	-22.65	-25.95	3	-7.22	-7.96	0.67	0.74
3	0.00	0.00	45.19	46.82	2	2	-16.30	-17.93	28.54	31.39	3	-6.61	-7.39	-2.97	-3.32	4	2.19	2.71	-1.27	-1.58
4	0.00	0.00	20.28	22.55	3	3	-32.14	-33.66	3.27	3.42	4	-0.19	-0.19	5.47	5.45	5	-6.10	-5.93	-0.09	-0.08
5	0.00	0.00	6.91	8.64	4	4	5.32	5.67	0.01	0.01	5	-5.81	-5.41	6.36	5.92	6	0.00	0.00	20.86	23.21
6	0.00	0.00	11.60	11.88	5	5	3.36	2.55	-3.98	-3.02	6	31.48	33.88	-0.00	-0.00	1	-0.08	-0.08	10.22	11.67
7	0.00	0.00	4.94	4.39	6	6	5.14	3.15	4.27	2.16	7	6.97	8.13	7.43	8.65	2	7.08	7.79	10.65	11.73
0	16.29	5.99	-0.00	-0.00	0	0	0.00	0.00	50.37	51.84	2	2.16	2.36	12.65	13.82	3	-3.83	-3.50	-2.42	-2.31
1	-53.02	-50.20	0.00	0.00	1	1	16.42	19.53	-8.29	-9.87	3	6.82	7.98	18.46	21.60	4	-2.83	-2.64	12.59	11.75
2	22.32	19.76	-0.00	-0.00	2	2	0.59	1.09	19.58	21.68	4	8.31	8.55	3.13	3.12	5	0.00	0.00	-5.72	-5.20
3	14.99	16.29	-0.00	-0.00	3	3	-0.74	-0.80	-15.73	-14.82	5	4.51	5.53	1.10	1.35	6	-0.00	-0.00	0.68	0.69
4	-25.94	26.18	-0.00	-0.00	4	4	-7.27	-7.49	-0.80	-0.82	6	3.95	3.21	1.05	0.85	1	10.70	11.84	0.68	0.69
5	7.16	8.04	-0.00	-0.00	5	5	0.96	0.87	-5.82	-5.24	7	8.57	9.42	0.00	0.00	2	2.45	2.95	3.10	3.73
1	-0.00	-0.00	-23.37	-23.22	0	0	-1.52	-1.34	6.14	5.42	1	15.25	17.65	3.57	4.24	3	5.30	5.62	0.96	1.02
2	-0.00	-0.00	-11.24	-12.26	0	0	-0.03	-0.00	-3.59	-3.39	2	-4.60	-3.36	-15.04	-15.40	4	-1.82	-1.71	3.38	2.81
3	-0.00	-0.00	-34.42	-34.75	1	1	15.80	16.97	-0.84	-0.91	3	3.81	4.34	4.33	4.90	0	-0.00	-0.00	-5.86	-6.60
4	-0.00	-0.00	-12.15	-13.03	2	2	-15.64	-16.88	-16.90	-18.22	4	-3.40	-2.94	-2.86	-2.47	1	-1.54	-1.51	-2.84	-2.80
5	-0.00	-0.00	-8.13	-8.74	3	3	27.19	29.68	0.99	1.08	5	3.01	2.66	-1.60	-1.42	2	0.33	0.35	-8.47	-8.31
6	-0.00	-0.00	-4.35	-5.02	4	4	4.21	3.93	-2.65	-2.47	6	-18.44	-19.47	0.00	0.00	3	1.95	1.75	-0.75	-0.68
0	-32.78	-32.77	0.00	0.00	0	0	-2.45	-1.57	-3.76	-2.41	1	-3.47	-3.46	-3.19	-2.18	1	-7.75	-3.18	-1.75	-1.65
1	18.15	23.37	-0.00	-0.00	1	1	-0.00	-0.00	-19.59	-18.05	2	2.63	2.95	-1.90	-1.67	2	-4.41	-3.60	-0.52	-0.42
2	2.13	2.63	0.00	0.00	2	2	4.76	5.44	-5.84	-6.68	3	-1.96	-2.47	-2.92	-3.26	3	0.00	0.00	43.19	40.00
3	-25.67	-25.97	0.00	0.00	3	3	2.40	2.25	-0.67	-0.24	4	-10.26	-10.47	1.91	1.95	4	-0.00	-0.00	-212.45	-159.30
4	-13.78	-14.53	0.00	0.00	4	4	2.40	2.25	-0.67	-0.24	5	0.35	0.33	2.69	2.54	5	-41.53	-40.06	0.00	0.00
5	-7.16	-7.33	0.00	0.00	5	5	2.40	2.25	-0.67	-0.24	6	1.18	0.93	5.53	4.38	6	2.71	2.67	0.00	0.00
6	-4.11	-4.01	0.00	0.00	6	6	-5.84	-4.89	5.11	4.28	7	-2.69	-1.35	0.00	0.00	7	-0.00	-0.00	-13.62	-15.57
1	0.00	0.00	3.61	3.34	0	0	-0.00	-0.00	4.22	4.65	0	-3.48	-3.22	-0.87	-0.80	1	-21.31	-17.63	80.36	73.12
2	0.00	0.00	16.02	18.28	1	1	-14.00	-16.44	6.61	7.77	2	2.17	1.77	-3.86	-3.52	2	-3.49	-3.78	-5.60	-6.05
3	0.00	0.00	11.60	10.43	2	2	5.99	6.03	3.21	3.23	3	0.25	0.79	-0.00	-0.00	3	6.62	6.91	-28.06	-29.32
4	0.00	0.00	1.93	3.17	3	3	-13.13	-14.78	-0.99	-1.11	4	-0.42	-0.09	2.57	0.53	4	-6.88	-6.49	-4.39	-4.10
5	0.00	0.00	2.89	3.49	4	4	-0.55	-0.65	2.77	3.25	5	0.00	0.00	-11.40	-11.11	5	-6.86	-7.43	25.95	28.14
6	0.00	0.00	3.21	3.86	5	5	-8.03	-6.32	-2.20	-1.73	6	76.53	69.41	-0.00	0.00	6	-27.53	-22.81	-0.00	-0.00
0	47.68	54.87	-0.00	-0.00	0	0	0.00	0.00	6.19	5.95	1	-0.00	-0.00	-16.98	-18.17	0	38.94	32.70	102.53	86.09
1	7.74	9.28	-0.00	-0.00	1	1	-0.30	-0.41	5.02	6.74	2	2.33	1.48	0.00	0.00	1	46.88	43.75	-30.72	-28.67
2	-5.95	-5.49	0.00	0.00	2	2	5.71	4.02	-2.40	-2.59	3	0.00	0.00	0.00	0.00	2	3.52	2.48	29.87	29.45
3	14.43	15.79	-0.00	-0.00	3	3	7.49	6.96	-0.33	-0.30	4	0.00	0.00	3.64	4	-8.02	-8.56	-3.04	-3.58	
4	1.79	1.05	-0.00	-0.00	4	4	7.32	8.00	-1.70	-1.86	5	23.61	19.74	58.19	82.10	5	3.99	3.63	11.61	12.41
5	3.77	4.49	-0.00	-0.00	5	5	5.71	4.02	-2.40	-2.59	6	15.08	13.39	-17.44	-15.62	6	1.95	2.07	8.21	8.72
1	-0.00	-0.00	5.45	5.32	0	0	-0.00	-0.00	10.01	9.35	1	21.13	21.67	-39.96	-40.57	7	1.25	1.41	4.24	4.12
2	-0.00	-0.00	-6.01	-5.27	1	1	-5.04	-4.61	-3.67	-3.35	2	5.74	6.49	15.10	17.08	8	-11.51	-11.20	-31.48	-30.64
0	-12.70	-13.77	0.00	0.00	2	2	-1.45	-1.39	-5.56	-5.32	3	5.73	2.79	-17.36	-17.44	9	23.11	22.96	-0.00	-0.00
1	-3.75	-3.83	0.00	0.00	3	3	60.08	60.07	7.21	7.36	4	5.07	5.09	1.53	1.53	10	-11.51	-11.20	-31.48	-30.64
2	-4.91	-5.79	0.00	0.00	4	4	90.37	66.45	0.00	0.00	5	0.03	0.03	-4.42	-4.72	11	38.47	37.12	14.48	13.98
3	3.41	2.32	-0.00	-0.00	5	5	0.00	0.00	-93.65	-74.63	6	3.03	3.03	0.00	0.00	12	-1.01	-1.19	2.33	3.09
1	-0.00	-0.00	-3.30	-2.56	6	6	37.74	36.25	0.00	0.00	7	0.00	0.00	18.95	15.56	13	21.65	22.84	-2.99	-3.16
2	-0.00	-0.00	-3.84	-2.91	7	7	36.08	34.07	0.00	0.00	8	47.58	41.88	10.51	9.16	14	13.57	13.61	-15.34	-15.13
3	-0.00	-0.00	-4.95	-3.74	8	8	-0.00	-0.00	10.57	-11.50	9	-37.58	-35.14	-4.19	-4.04	15	4.06	4.83	8.03	8.19
0	-5.16	-4.48	0.00	0.00	9	9	8.57	8.04	-0.00	-0.00	10	-11.80	-13.13	9.95	11.07	16	2.90	3.70	-1.19	-1.19
1	-4.50	-2.12	0.00	0.00	10	10	-133.30	-95.31	0.00	0.00	11	5.13	12.73	-0.51	-0.57	17	-8.86	-9.00	0.00	0.00
1	0.00	0.00	-28.70	-20.76	2	2	-28.75	-21.07	39.49	35.86	12	-9.30	-10.03	2.50	2.53	18	-27.29	-25.03	-8.51	-7.80
2	6.51	6.55	0.00	0.00	3	3	3.14	11.79	-27.83	-18.93	13	0.00	0.00	-28.47	-26.66</					

1	-6.22	-7.11	-16.77	-19.17	1	4.09	4.19	-24.04	-24.63	3	5.76	4.73	-1.28	-1.05					h10	l=12	
2	-3.35	-3.11	12.99	12.04	2	-5.52	-5.87	-7.86	-8.36	4	-2.61	-2.45	-5.17	-4.83	0	7.53	7.28	-0.00	-0.00		
3	31.62	33.24	18.49	20.07	3	1.88	1.96	-17.02	-17.78	5	3.72	5.17	1.19	1.66	1	0.83	0.55	2.98	3.07		
5	3.32	-2.23	-3.89	-2.62	4	2.06	1.99	-6.76	-6.50	0	-0.00	h8	l=11	-11.33	-12.68	0	-7.67	-5.51	0.00	0.00	
6	-5.96	-6.42	1.31	1.41	5	-3.21	-2.97	-5.45	-5.05	1	-12.31	-12.33	6.03	6.03	1	-0.00	-0.00	-11.53	-15.17		
0	-0.00	-0.00	-11.49	-10.16	0	-14.61	-15.15	0.00	0.00	3	-2.15	-1.77	3.09	2.55	2	-0.00	-0.00	-25.24	-25.21	0.00	0.00
1	13.46	13.66	-11.35	-14.56	1	-7.14	-7.75	-5.98	-6.49	4	-1.74	-2.02	-2.88	-3.34	3	-0.00	-0.00	26.18	27.82		
2	-5.84	-1.19	-27.25	-26.86	2	-7.08	-6.48	-11.97	-10.96	2	0.00	h10	l=11			5	0.00	0.00	10.57	14.96	
3	-7.08	-6.48	-11.97	-10.96	2	-13.31	-13.04	4.62	4.53	0	0.00	0.00	8.21	7.00				h1	l=11		
4	-2.78	-2.89	-14.98	-15.59	3	-4.36	-3.42	-0.98	-0.77	1	-8.66	-9.91	-1.68	-1.93	0	-0.00	-0.00	7.22	7.65		
5	-1.27	-1.22	9.38	9.03	4	-5.49	-5.76	0.35	0.37	2	1.09	1.03	5.23	4.92	1	-11.39	-11.37	-52.77	-52.67		
6	-2.45	-2.44	-0.33	-0.33	5	-5.49	-5.76	0.35	0.37	2	-5.40	-4.79	-1.12	-0.99	2	60.50	65.81	-14.88	-16.18		
1	-30.50	-31.60	11.19	11.59	0	11.64	11.66	-0.00	-0.00	4	-0.60	-0.63	2.62	2.73	3	-3.50	-3.89	21.66	24.07		
2	1.07	1.13	-24.25	-25.75	1	5.42	5.35	10.05	9.92	0	h11	l=11			4	-7.68	-9.36	-6.35	-7.73		
3	-13.28	-13.19	-5.30	-5.26	2	-0.94	-1.05	3.02	3.35	0	0.00	0.00	5.09	6.22	5	-5.12	-4.72	-1.86	-1.72		
4	-1.57	-1.34	-4.33	-3.71	3	-3.46	-2.44	-2.53	-1.79	1	5.24	5.44	-2.24	-2.33	6	9.51	9.60	0.04	0.04		
5	4.82	4.77	-0.54	-0.54	5	1.70	1.32	0.81	0.63	2	-0.75	-0.89	6.80	6.42				h2	l=13		
6	4.82	4.77	-0.54	-0.54	5	1.70	1.32	0.81	0.63	2	4.73	4.27	1.24	1.11	0	-0.00	-0.00	-13.69	-12.97		
0	0.00	0.00	13.24	13.21	2	-2.22	-2.27	6.43	6.56	0	h12	l=11			1	46.33	44.47	20.56	19.74		
1	-6.32	-6.66	-11.76	-12.38	3	6.47	6.70	-2.56	-2.65	0	-0.00	-0.00	-3.01	-3.05	2	3.68	2.98	1.87	-3.13		
2	-1.33	-1.37	13.40	13.87	4	5.32	4.98	-6.81	-6.38	1	3.78	3.53	1.76	1.65	3	-9.28	-9.63	-18.59	-19.70		
3	8.41	7.79	10.34	9.59	4	3.29	1.82	2.23	1.24	0	71.24	68.99	-0.00	-0.00	5	-4.20	-2.41	17.20	18.81		
4	1.87	1.53	-1.03	-3.29	1	-4.03	-3.60	4.03	3.61	1	-0.00	-0.00	20.89	17.65				h3	l=13		
5	0.00	0.00	3.52	2.58	2	-0.32	-0.32	-1.93	-1.90	2	-15.37	-16.17	-0.00	-0.00	1	15.37	17.93	29.59	34.52		
6	27.49	28.46	-10.07	-10.42	3	0.84	0.46	-1.91	-1.03	3	-0.00	-0.00	-8.80	-8.11	2	-25.44	-27.75	9.21	10.05		
0	-1.25	-1.17	8.91	8.32	0	h11	l=10			4	31.86	33.96	-0.00	-0.00	3	17.76	17.93	-8.72	-8.81		
1	10.97	10.77	-1.55	-1.53	0	7.72	6.96	-0.00	-0.00	5	0.00	0.00	7.00	7.58	4	-2.79	-3.26	8.43	9.84		
2	-0.33	-0.31	2.97	2.77	1	h12	l=10			6	3.01	3.24	-0.00	-0.00	5	4.74	4.02	-2.41	-2.04		
3	5.38	5.10	2.25	2.13	1	-0.73	-0.57	-6.69	-5.18	0	-18.64	-20.87	0.00	0.00	6	-8.20	-8.66	-1.12	-1.18		
4	-0.00	-0.00	-15.97	-16.98	1	-0.00	-0.00	35.09	29.53	1	-5.75	-5.46	-32.19	-49.50	0	0.00	0.00	-5.56	-9.17		
5	2.44	2.55	6.35	6.63	2	-10.19	-11.28	0.00	0.00	2	52.81	56.82	2.23	2.40	1	-1.04	-1.22	-18.86	-22.28		
6	1.63	2.07	-1.01	-4.58	3	-0.00	-0.00	2.13	0.79	3	-3.87	-4.22	-40.09	-43.78	2	20.12	22.33	-11.86	-13.16		
0	6.81	6.20	0.39	0.54	4	-23.29	-23.83	0.00	0.00	4	4.93	4.22	4.04	3.16	3	-5.59	-5.08	3.33	3.02		
1	-2.61	-2.77	-0.54	-5.35	5	0.00	0.00	10.43	10.39	0	h10	l=8			4	0.13	0.13	-12.54	-12.80		
2	-10.73	-11.68	3.04	3.31	0	-6.44	-5.65	0.00	0.00	1	0.53	0.51	6.26	5.94	5	0.57	0.61	6.17	6.66		
3	1.66	1.89	-1.02	-1.17	1	0.00	0.00	-5.52	-1.74	3	2.75	1.88	-2.71	-1.85				h5	l=13		
4	-12.56	-11.22	-1.11	-0.99	2	-32.97	-31.22	76.26	72.22	3	0.03	0.02	-3.03	-1.93	1	-12.05	-12.59	-15.70	-16.41		
5	-0.24	-0.20	-2.28	-1.96	3	12.40	12.11	-7.68	-7.70	5	0.70	0.68	-1.57	-1.45	2	13.60	14.84	-16.30	-17.79		
6	0.00	0.00	7.58	8.56	5	6.31	6.12	11.92	11.55	6	-3.52	-2.90	-2.49	-2.05	3	-27.85	-29.07	5.36	5.60		
0	-2.52	-2.13	-0.42	-0.35	6	-3.74	-4.31	-9.19	-10.59	7	h2	l=12			4	3.61	3.28	0.16	0.14		
1	0.76	0.73	7.09	6.78	6	-6.97	-7.11	5.06	5.17	0	-21.94	-22.52	0.00	0.00	5	1.30	1.46	4.34	3.55		
2	-2.94	-2.87	1.10	1.07	0	5.89	6.81	-0.58	-0.68	1	-20.05	-17.12	-10.17	-8.68	6	7.05	6.54	12.27	2.10		
3	-0.00	-0.00	2.29	1.10	1	0.00	0.00	-6.01	-5.82	2	-4.01	-2.88	5.41	3.89	0	0.00	0.00	34.37	38.36		
4	3.54	4.18	0.42	0.49	2	18.34	16.33	-11.33	-10.09	4	-8.43	-8.36	5.75	5.70	1	-19.43	-20.67	10.15	10.78		
5	-22.68	-21.57	0.00	0.00	4	7.61	7.54	-10.33	-10.24	5	-22.00	-22.51	-4.62	-4.73	2	-18.02	-18.85	15.04	15.73		
6	0.00	0.00	33.24	32.95	5	-5.98	-5.84	-2.89	-2.82	1	-0.20	-0.38	32.12	29.23	3	8.50	8.54	-0.11	-0.11		
0	44.96	45.83	-0.00	-0.00	6	13.08	12.25	1.52	1.43	2	-0.64	-0.65	-10.55	-10.62	3	4.16	3.83	5.68	5.23		
1	0.00	0.00	10.57	8.90	0	-10.15	-10.21	-8.57	-8.62	3	2.96	3.18	47.43	50.96	4	-2.47	-2.17	-5.90	-5.18		
2	0.00	0.00	6.33	6.61	0	5.89	6.37	-0.37	-0.40	4	-5.11	-5.76	-0.25	-0.28	5	0.00	0.00	7.07	7.00		
3	0.00	0.00	4.22	4.00	0	0.00	0.00	-9.80	-7.53	5	-0.52	-0.63	2.92	3.53	2	14.43	14.81	5.61	5.76		
4	0.00	0.00	3.37	3.05	3	27.92	27.41	-18.30	-17.97	0	5.90	7.02	-0.00	-0.00	4	-12.79	-12.98	-13.07	-13.26		
5	99.93	89.43	-0.00	-0.00	4	-3.23	-3.46	28.18	31.79	1	-8.58	-9.38	5.78	6.32	3	0.00	0.00	-26.30	-27.10		
6	-14.95	-13.55	42.33	38.36	5	3.87	3.20	1.84	1.53	2	13.68	13.18	7.35	6.98	0	-0.00	-0.00	-4.42	-4.42		
0	54.04	53.71	-20.71	-20.05	6	-6.82	-7.41	-15.11	-16.42	3	16.37	16.60	-0.00	-0.00	1	8.98	8.99	-4.42	-4.42		
1	-8.27	-9.86	-14.24	-16.97	5	8.15	7.87	-13.16	-12.71	4	6.44	7.03	4.69	4.88	2	0.28	0.28	-11.55	-11.30		
2	27.53	29.67	4.43	4.77	0	-3.32	-3.54	1.42	1.51	5	6.89	3.59	11.21	10.34	3	-4.06	-3.57	1.86	1.64		
3	3.38	2.90	-4.78	-4.10	1	-0.00	-0.00	3.59	3.96	6	1.43	1.66	2.01	2.33	4	-1.51	-1.46	-7.75	-7.52		
4	28.72	27.14	-0.00	-0.00	2	3.74	2.59	0.77	0.53	0	-5.21	-6.71	0.00	0.00	1	-12.94	-13.30	0.20	0.20		
5	-59.91	-52.37	-33.98	-29.70	3	-0.33	-0.33	-17.72	-18.73	1	20.39	20.55	-17.38	-17.51	2	5.84	5.07	2.71	2.35		
6	-45.73	-33.22	-23.05	-24.66	4	3.52	2.61	4.88	3.62	2	9.44	10.43	-18.40	-20.33	3	-5.40	-5.76	0.93	0.99		
0	6.90	7.50	-40.75	-44.28	5	6.89	5.87	6.17	5.26	3	5.58	5.75	-28.26	-29.13	4	-1.60	-1.18	2.62	1.94		
1	1.71	1.51	5.20	4.59	6	-6.01	-6.30	-1.04	-1.09	5	2.38	2.59	-1.76	-1.91	5	-1.60	-1.18	2.62	1.94		
2	0.97	0.97	-6.77	-6.78	0	-0.00	-0.00	-8.62	-8.33		1.55	1.59	-2.39	-2.46	0	0.00	0.00	11.15	10.94		
3	-2.03	-1.92	-6.61	-6.24	1	-6.45	-8.67	-0.55	-0.59	0	-30.58	-32.18	0.00	0.00	1	3.06	3.18	8.17	8.50		
4	-15.66	-16.43	0.00	0.00	3	8.83	9.72	-38.53	-42.41	1	12.72	13.86	-12.73	-13.87	2	-0.00	-0.00	-1.95	-1.25		
5	17.33	17.21	-5.00	-4.96	4	-8.89	-8.66	-2.86	-2.79	2	-0.63	-0.65	-11.63	-12.01	1	7.94	7.65	-0.32	-0.31		
6	-22.05	-23.97	20.90	22.71	5	0.61	0.71	-4.94	-5.70	3	-11.87	-11.72	-0.08	-0.07	0	46.06	47.50	-0.00	-0.00		
0	-0.30	-0.37	-3.82	-4.70	6	-1.10	-0.97	12.38	10.90	4	-4.26	-4.55	-2.07	-2.21	1	-0.00	-0.00	-41.80	-43.64		
1	-7.70	-7.45	-6.42	-6.22	0	3.98	3.46														

5	-1.57	-1.93	1.07	2.30	h=3	1=21			h=10	1=22	3	-0.00	-0.00	11.78	11.73					
0	-0.00	-0.00	-8.75	-9.57	1	2	-3.87	-4.80	5.64	6.99	1	-0.51	-0.37	-2.42	-1.05	4	-12.07	-10.00	0.00	0.00
1	-13.28	-12.73	-7.55	-7.24	3	4	0.86	0.83	-12.29	-11.81	2	1.69	5.07	-0.00	-0.00	1	8.27	-3.84	8.54	10.13
2	-1.74	1.31	-3.44	-2.60	4	4	7.00	7.48	1.98	2.10	3	-0.00	-0.00	-7.87	-8.50	1	-0.45	-0.45	-1.82	-1.82
3	-10.15	-9.56	2.96	2.78	5	5	-3.96	-3.77	-1.18	-1.11	4	-12.81	-11.44	0.80	0.00	2	-0.45	-0.45	-3.61	-3.61
4	3.87	3.31	1.44	-1.23	0	0	-0.00	-0.00	11.42	12.44	5	0.00	0.00	0.20	6.54	3	0.91	0.91	17.30	19.26
0	0.00	0.00	10.77	11.42	1	1	12.19	12.11	-16.01	-13.90	1	-12.67	-13.83	9.48	10.35	1	-5.35	-4.04	-12.95	-12.02
1	-4.21	-3.30	-3.29	-2.58	4	4	-0.04	-0.04	13.19	13.92	3	5.15	4.98	3.27	2.17	3	5.66	5.67	8.67	0.59
2	1.15	1.32	6.22	7.15	2	2	-11.00	-10.04	1.50	1.37	3	h=10	1=23	9.48	10.35	5	1.24	1.11	-4.88	-6.24
4	1.76	1.47	6.23	6.87	5	5	1.66	1.57	-5.69	-5.40	1	-12.67	-13.83	9.48	10.35	5	5.15	4.99	3.27	3.17
0	-0.00	-0.00	-2.96	-1.60	0	0	-0.00	-0.00	-15.35	-18.57	4	5.15	4.99	3.27	3.17	0	-0.00	-0.00	4.56	4.10
1	10.52	10.09	0.66	0.63	2	2	13.95	14.50	2.68	2.79	5	1.29	1.41	1.87	2.04	0	7.81	9.33	-1.02	-1.22
3	7.65	7.40	1.00	-0.97	3	3	2.63	3.02	-0.81	-0.76	1	-3.08	-2.97	9.90	9.52	1	h=3	1=25	h=3	1=25
0	-0.00	-0.00	-5.05	-5.38	4	4	-3.49	-3.57	6.10	6.24	1	-5.71	-7.47	2.01	2.63	2	-8.96	-9.81	0.77	0.83
1	3.25	2.38	-2.83	-2.07	5	5	-3.05	-3.35	-5.69	-5.78	2	4.99	5.77	-2.51	-2.91	3	2.84	2.45	-0.68	-0.59
2	-0.60	-0.61	-6.14	-6.29	1	1	4.38	3.84	-0.40	-0.35	3	-9.74	-9.41	4.10	3.97	3	h=4	1=25	h=4	1=25
0	-24.10	-27.88	-8.00	-0.00	2	2	-1.25	-1.27	9.11	9.25	4	8.73	7.60	-1.78	-1.55	0	-0.00	-0.00	-10.75	-15.18
1	-0.00	-0.00	16.56	14.14	3	3	0.81	0.77	-14.90	-14.25	5	-2.14	-2.00	-4.72	-4.42	0	8.78	8.25	-5.55	-5.22
2	-43.03	-46.65	0.00	0.00	4	4	-7.07	-6.97	3.11	3.06	1	15.95	16.23	-10.69	-10.83	2	-10.33	-8.68	-2.52	-2.12
4	-7.76	-8.39	0.00	0.00	5	5	4.49	4.31	-2.00	-1.92	3	-4.47	-4.77	-0.74	-0.79	3	-0.21	-0.20	8.73	8.60
5	0.00	0.00	13.31	13.38	1	1	-2.19	-2.14	2.47	2.41	4	-8.78	-7.23	-1.96	-1.61	4	-0.21	-0.20	-3.00	-3.07
6	-4.44	-4.33	0.00	0.00	0	0	0.00	0.00	16.33	17.21	5	3.87	3.94	-5.97	-6.08	0	0.00	0.00	-6.55	-6.07
1	18.05	20.31	25.22	32.87	2	2	-13.37	-13.55	-5.64	-5.50	0	0.00	0.00	13.19	1.82	1	-9.91	-10.57	-0.81	-0.66
2	11.54	12.46	-3.62	-3.91	4	4	-3.92	-3.57	7.70	7.02	2	-11.68	-12.04	-4.25	-4.38	2	6.73	6.87	-0.00	-0.05
5	0.03	0.08	7.40	7.78	4	4	4.69	4.27	5.73	5.21	3	10.34	9.37	-0.79	-0.72	3	-3.92	-8.05	-1.36	-1.38
6	2.76	2.27	-2.53	2.09	1	1	h=8	1=21	h=8	1=21	4	-3.10	-3.16	-0.53	-0.54	4	-0.34	-0.29	-3.02	-3.09
1	-1.45	-2.35	-10.91	-13.12	3	3	2.85	2.55	-4.41	-3.95	0	-0.00	-0.00	-2.56	-3.55	0	0.00	0.00	-4.80	-6.91
2	25.19	30.77	-3.24	-4.41	4	4	3.37	2.93	7.22	6.37	1	0.45	0.44	9.50	9.41	1	-6.46	-7.98	4.54	4.55
3	-3.68	-3.93	-3.93	-4.32	0	0	-0.00	-0.00	-10.25	-10.43	4	0.97	1.03	-11.40	-11.37	2	5.55	5.21	6.23	5.82
4	4.94	5.30	0.67	0.72	1	1	7.21	7.51	-0.70	-0.72	5	5.20	4.38	-3.97	-3.01	3	1.56	1.26	-4.78	-4.53
5	4.47	4.09	-4.43	-8.62	2	2	2.08	2.03	-4.75	-4.64	1	-12.40	-12.83	2.65	2.74	4	2.13	1.66	0.08	3.30
6	3.05	3.94	0.07	0.09	3	3	5.68	4.58	0.97	0.78	2	4.44	4.60	5.81	6.02	0	0.00	0.00	3.50	3.31
1	-22.95	-25.21	-26.16	-23.72	4	4	-0.00	-0.00	-3.14	-3.51	4	-10.12	-8.93	1.91	1.62	1	6.92	6.56	-4.07	-3.90
2	-13.85	-13.60	3.89	3.91	1	1	-5.35	-4.62	0.62	0.53	3	4.13	3.66	2.41	2.12	2	-2.14	-1.76	4.25	3.52
3	0.10	-0.11	-12.34	-12.37	0	0	-16.87	-16.77	0.00	0.00	1	-1.19	-1.11	-3.31	-3.09	0	-0.00	-0.00	-4.92	-4.83
4	4.04	4.17	-6.42	-6.64	0	0	0.00	0.00	21.52	24.60	4	0.24	0.20	6.39	5.94	1	6.17	6.73	-4.08	-3.95
5	0.48	1.40	11.03	11.21	1	1	-18.40	-18.88	0.00	0.00	5	5.60	6.90	-5.14	-6.10	2	-0.94	-0.90	-4.95	-5.21
1	-9.50	-9.23	7.08	6.93	3	3	0.00	0.00	0.00	0.00	2	1.96	1.23	-3.91	-2.48	0	-3.00	-6.00	-2.60	-1.75
2	-10.03	-11.10	-10.92	-12.06	4	4	-3.83	-3.58	0.00	0.00	3	9.67	8.90	-0.66	-0.61	1	-6.60	-6.12	3.50	3.24
3	0.39	0.36	5.21	4.80	5	5	0.38	0.00	4.02	4.61	3	h=9	1=23	h=9	1=23	3	4.94	4.22	0.00	0.00
4	-2.69	-2.74	5.20	5.28	0	0	56.76	67.17	-0.00	-0.00	0	-0.00	-0.00	-8.05	-7.15	0	-0.00	-0.00	5.74	6.83
5	-6.00	-5.32	5.24	4.64	0	0	-4.91	-5.68	1.58	1.62	1	-4.56	-3.70	-1.69	-1.57	1	11.98	10.04	-0.00	-0.00
0	3.95	5.46	-0.00	-0.00	3	3	2.62	2.90	-8.13	-8.78	2	-0.09	-0.10	-5.94	-6.12	2	0.00	0.00	2.89	2.82
1	4.38	4.60	16.31	19.21	4	4	14.39	14.93	1.05	1.09	0	31.66	33.34	-0.00	-0.00	3	-0.00	-0.00	0.73	-0.77
2	0.87	5.50	6.77	5.22	1	1	-25.19	-25.81	-15.70	-16.09	1	0.00	0.00	34.57	40.64	1	-5.71	-3.56	-10.20	-11.70
3	-2.83	-1.17	-11.69	-11.61	2	2	10.56	10.92	0.82	0.85	4	14.79	14.98	-0.48	-0.46	2	-5.71	-3.78	-3.16	-3.16
4	-2.10	-2.10	5.72	2	2	0.19	0.20	-14.47	-15.09	5	0.00	0.00	4.08	4.65	2	0.73	0.73	-20.61	-20.74	
5	0.11	0.10	8.44	7.42	3	3	8.90	5.51	-1.16	-1.10	3	-8.37	-9.35	-8.41	-9.37	3	1.90	1.19	-0.82	-5.14
1	6.14	6.43	-4.82	-5.04	4	4	2.63	2.47	-4.32	-4.24	1	20.27	21.70	-3.68	-3.50	3	-13.11	-13.10	3.78	3.77
2	6.13	6.47	6.89	8.94	5	5	-35.72	-43.77	0.00	0.00	3	-1.50	-1.39	-5.52	-5.14	2	-0.97	-0.67	-4.31	-2.97
3	3.27	3.01	-2.29	-2.11	0	0	8.47	9.22	5.41	5.89	5	4.46	4.03	-6.30	-5.70	3	-3.55	-3.37	3.06	2.90
4	4.05	4.14	-4.48	-4.58	1	1	-4.28	-6.19	-0.69	-1.00	4	-1.61	-1.63	-23.41	-22.73	5	-5.64	-3.23	4.47	3.96
5	2.55	3.59	-4.39	-4.14	2	2	-7.45	-6.98	-2.11	-1.58	2	-7.87	-7.73	4.08	4.01	4	6.38	6.79	9.23	9.81
1	-4.03	-3.59	-9.91	-8.83	4	4	-5.18	-4.30	-2.28	-1.68	4	-10.89	-9.97	6.98	-2.73	1	9.67	9.45	5.47	5.34
2	-1.20	-2.10	-7.87	-7.26	5	5	1.44	0.43	9.55	9.30	1	4.42	4.39	11.00	11.46	3	-1.72	-1.70	14.45	14.37
4	-0.57	-1.04	-1.63	-2.94	1	1	-3.44	-4.02	-1.93	-1.79	2	-17.89	-18.21	4.59	5.08	4	-3.89	-2.29	1.60	1.11
0	-4.37	-4.34	1.28	1.27	2	2	-2.24	-2.16	11.96	11.44	3	2.34	1.73	4.26	2.90	5	-1.52	-1.39	4.18	3.04
1	-4.82	-3.82	0.82	0.68	3	3	-6.70	-5.94	5.34	4.73	4	-2.76	-3.36	1.45	1.77	1	0.00	0.00	2.89	2.82
2	-4.83	-3.98	2.18	1.80	4	4	-0.32	-0.31	3.70	3.64	5	-7.29	-5.99	2.79	2.29	0	14.47	16.55	-0.00	-0.00
3	-3.03	-0.56	-0.00	-0.00	5	5	h=5	1=22	h=5	1=22	1	-2.99	-4.08	3.25	4.41	1	1.94	1.77	-1.26	-8.10
4	7.30	5.60	2.65	2.03	0	0	21.34	21.22	-0.00	-0.00	2	13.64	13.99	-3.44	-3.49	3	11.05	10.61	0.82	0.79
5	0.33	0.32	3.78	3.73	1	1	-2.64	-2.47	-2.97	-2.78	2	3.88	4.23	-6.83	-7.44	4	3.77	3.37	4.82	4.85
0	-0.71	-0.39	0.00	-2.75	2	2	8.21	8.22	8.13	8.14	3	6.23	5.18	6.93	7.73	5	1.55	2.71	-2.92	-3.97
1	0.29	2.07	-0.00	-0.00	3	3	6.87	6.90	5.85	5.84	4	6.23	5.18	6.93	7.73	1	h=5	1=26	h=5	1=26
2	-0.94	-0.38	-2.50	-1.01	5	5	7.50	5.86	2.81	2.15	5	0.93	1.11	-1.84	2.21	2	-0.76	-0.75	-4.08	-3.97
0	-0.00	-0.00	-15.66	-15.59	0	0	-6.66	-6.24	-0.00	-0.00	2	10.31	10.68	-9.30	-8.39	3	-3.04	-2.82	-6.13	-5.67
1	23.65	27.31	-0.00	-0.00	1	1	15.96	15.01	-5.32	-5.22	4	4.97	4.89	-0.81	-0.67	4	2.73	2.44	-10.97	-1.83
2	0.00	0.00	-3.84	-2.69	2	2	5.56	4.19	-0.72	-0.54	1	-13.38	-12.84	-1.53	-1.72	4	3.33	1.92	-1.55	-0.

2	2.45	2.30	-0.00	0.00	3	3.75	3.14	1.25	1.04	4	-5.60	-4.99	-1.63	-1.44	3	2.47	2.69	1.94	2.12
4	4.38	3.93	0.00	0.00	4	5.93	5.33	2.79	2.50	1	6.85	6.60	5.11	4.98	0	6.57	5.16	-0.00	-0.00
5	0.00	0.00	5.65	6.05	0	4.31	6.19	-0.00	-0.00	2	8.09	7.69	1.95	1.50	1	-1.41	-1.39	-0.57	-0.24
2	3.29	3.83	2.42	2.01	1	-2.68	-2.52	-11.70	-11.62	3	2.94	2.49	8.22	6.97	2	-7.11	-3.29	-5.48	-4.07
4	4.05	3.88	2.62	2.51	2	2.71	2.55	-9.12	-8.81	4	6.46	4.96	3.80	2.98	3	2.64	2.62	-5.45	-3.49
1	-0.96	-0.92	-14.55	-11.94	4	3.16	2.99	-9.87	-9.34	1	6.05	5.67	-4.94	-4.79	0	-7.79	-7.56	0.00	0.00
2	-1.09	-1.14	9.81	10.26	0	-11.71	-12.33	0.00	0.00	2	10.69	11.07	-2.94	-3.05	2	-6.53	-6.77	-3.19	-0.51
3	-3.06	-2.79	-0.71	-0.64	0	3.90	3.81	-0.33	-0.35	0	3.16	3.37	1.03	1.10	3	-2.19	-2.17	-0.98	-0.98
4	-6.47	-4.25	4.44	0.45	1	-0.73	-0.70	-0.33	-0.35	0	-8.64	-8.62	0.00	0.00	1	0.23	0.23	4.13	6.16
1	5.65	6.16	1.24	1.36	2	-3.57	-3.03	-2.93	-2.35	1	-2.87	-2.45	-10.63	-9.26	2	4.45	3.16	3.12	2.22
2	-7.85	-6.92	-6.70	-5.91	1	0.46	0.40	8.42	7.39	3	-3.97	-4.98	-4.83	-3.95	0	h=6	l=32		
3	2.16	2.39	4.49	4.59	1	-4.96	-3.94	1.89	1.63	0	-2.60	-2.25	-4.43	-3.68	0	4.17	4.73	-0.00	-0.00
4	-1.17	-0.77	-1.11	-1.68	2	-4.47	-3.57	7.57	6.04	1	-4.56	-6.73	3.64	3.78	1	0.00	0.00	-2.69	-3.29
1	-0.34	-0.34	3.58	5.59	1	-3.10	-1.18	-8.16	-1.57	2	-3.94	-5.32	-1.90	-1.82	1	-3.34	-2.80	8.23	6.90
2	0.17	0.26	-10.92	-9.76	1	0.69	0.71	8.42	1.92	1	-0.62	-0.57	4.31	3.98	3	-3.01	-2.40	1.84	1.47
3	-3.06	-3.17	0.74	0.77	2	-0.00	-0.00	-19.36	-17.88	2	4.19	3.38	3.01	2.43	1	3.61	3.32	-5.65	-5.15
1	-8.55	-8.11	-0.11	-0.11	1	0.00	0.00	8.55	8.50	1	2.95	3.23	-1.79	-1.96	2	-0.82	-0.91	5.19	5.74
2	6.33	6.75	4.99	4.12	2	12.56	12.85	-6.00	-0.00	0	0.00	0.00	7.05	-5.53	0	0.00	0.00	2.94	1.64
3	-1.69	-2.62	-1.09	-2.79	3	-4.47	-3.57	7.57	6.04	1	0.00	0.00	-6.30	-5.61	1	3.58	4.16	1.10	1.57
4	-0.67	-0.61	4.16	3.61	2	8.83	8.22	3.73	3.63	3	6.62	5.97	-0.00	-0.00	0	7.85	7.14	0.00	0.00
0	0.00	0.00	7.36	6.85	1	1.11	1.06	9.81	9.36	4	h=1	l=31			0	0.00	0.00	0.00	0.00
1	3.72	3.54	-2.96	-2.82	2	-10.43	-9.79	-8.25	-8.20	3	4.68	3.91	-4.61	-4.02	1	0.00	0.00	0.00	0.00
2	0.11	0.60	8.83	8.30	3	3.98	4.45	-3.01	-3.60	4	2.57	1.60	1.77	1.10	2	-4.29	-4.15	0.00	0.00
3	6.22	5.85	-1.27	-1.10	3	h=3	l=29			4	h=2	l=31			3	0.00	0.00	0.00	0.00
1	5.75	5.27	-1.89	-1.73	2	-3.70	-3.25	-7.20	-6.50	3	-0.24	-0.21	0.91	0.08	1	h=1	l=34		
2	-3.00	-3.18	-1.84	-1.94	4	3.65	2.70	-3.96	-2.94	1	-3.24	-3.31	3.87	5.63	2	-0.77	-0.66	10.31	10.68
3	4.85	3.44	-0.59	-0.31	2	6.29	5.73	4.03	3.75	2	2.71	2.55	-2.36	-2.27	0	3.06	2.62	-1.79	-1.91
1	-6.20	-4.20	2.86	3.21	3	-6.73	-4.59	4.44	4.59	3	-9.52	-7.03	3.14	2.32	1	1.40	1.44	-7.02	-7.21
2	-0.56	-0.79	-6.96	-8.15	0	0.00	0.00	10.37	11.05	3	h=5	l=31			2	3.21	4.24	-2.26	-2.59
0	11.42	11.97	-8.03	-0.00	2	0.00	1.03	4.36	4.90	0	-1.08	-0.31	-6.28	-4.72	1	0.98	0.91	-8.00	-7.45
1	-1.00	-0.00	-6.36	-6.11	0	0.00	0.00	0.00	0.00	0	0.00	0.00	7.67	7.06	2	-2.07	-2.83	0.58	0.81
2	0.00	0.00	-0.00	-0.00	1	0.00	0.00	0.6	0.89	1	3.76	3.26	-3.93	-3.40	1	-2.28	-2.28	6.17	6.15
3	-0.00	-0.00	-0.00	-18.74	1	-4.17	-4.82	-2.83	-1.93	0	h=6	l=31			2	-4.18	-3.74	2.18	1.99
0	-1.98	-1.28	0.00	0.00	2	6.82	6.17	-2.57	-2.32	2	-0.00	-0.00	-3.77	-4.55	0	h=5	l=34		
1	-4.00	-4.13	-4.93	-4.69	0	-0.00	-0.00	-7.72	-8.15	0	0.33	0.26	-4.01	-3.86	1	-0.33	-0.36	4.93	4.53
2	-3.01	-3.12	1.73	2.35	0	-1.45	-1.57	-3.19	-4.31	0	-0.00	-0.00	-3.04	-4.13	2	2.93	3.23	-0.35	-0.28
4	-1.43	-1.69	-1.85	-1.87	0	h=4	l=29			1	-8.01	-8.69	0.00	0.00	1	1.96	3.59	1.51	2.74
0	-9.01	-11.76	0.00	0.00	0	0.00	8.00	3.43	1.31	2	-13.13	-11.70	0.00	0.00	0	5.05	4.00	-0.00	-0.00
1	1.43	1.59	10.43	11.28	0	11.80	10.31	-0.00	-0.00	3	-0.00	-0.00	-4.18	-3.78	1	0.00	0.00	7.45	7.10
2	-1.61	-1.74	3.63	6.44	0	-7.49	-7.00	0.00	0.00	0	-17.12	-14.20	0.00	0.00	1	-0.19	-0.26	-4.18	-6.09
3	-1.30	-1.1	11.26	11.93	2	-3.06	-0.00	10.33	-10.36	1	1.00	1.45	3.43	4.98	0	h=3	l=36		
4	-2.91	-3.17	0.40	0.45	3	-8.04	-7.92	0.00	0.00	2	1.23	-1.37	-10.51	9.80	0	-7.85	-6.39	0.00	0.00
0	15.81	17.51	-0.00	-0.00	0	-7.11	-7.42	0.00	0.00	3	-1.55	-1.37	-10.51	9.80	1	-1.68	-2.34	1.27	1.77
1	2.75	3.06	4.07	4.57	0	-3.69	-3.90	3.94	5.35	0	7.83	8.72	-0.00	-0.00	1	h=1	l=37		
2	2.44	2.89	-1.43	-1.71	2	-21.09	-19.15	3.43	3.30	2	11.45	10.02	-4.33	-3.70	1	-1.35	-0.91	3.07	3.41

parameters are listed in Table II with their estimated standard deviations. The observed and calculated structure factors are listed in Table III.

DESCRIPTION AND DISCUSSION OF THE STRUCTURE

The bond lengths and angles are collected in Table IV. The chlorpropamide molecule, with the labeling of atoms, is shown in Fig. 1. The benzene ring is lightly distorted from regular hexagon. Ring C-C bond lengths vary from 1.368 to 1.391 Å with the average

1.379 Å. The bond angles at benzene ring vary from 118.7 to 121.7°. It has been pointed out by many authors, namely, Klug²⁵, Arona and Sundaralingam²⁶ etc., that there is a tendency of stabilization of p-substituted benzene ring with the distortion from regular hexagonal form. The C(4)-Cl bond length is 1.728 Å long, in good agreement with the corresponding bond lengths (1.727 and 1.7374 Å) in N'-N-bis(3,4-dichlorophenyl) urea²⁷. The S-C(1) bond length 1.758 Å is in good agreement with the theoretical S-C(sp²) value(1.75 Å) calculated from the atomic radii and electronegativities given

Table IV: Bond lengths and angles in chlorpropamide.

a) Bond lengths in Å							
Cl	C(4)	1.728(9)		C(8)	C(9)	1.497(12)	
S	C(1)	1.758(6)		C(9)	C(10)	1.504(13)	
C(1)	C(2)	1.391(11)		C(2)	H1	1.01(5)	
C(2)	C(3)	1.378(13)		C(3)	H2	1.16(5)	
C(3)	C(4)	1.378(13)		C(5)	H3	1.06(5)	
C(4)	C(5)	1.370(11)		C(6)	H4	1.09(5)	
C(5)	C(6)	1.368(12)		N(1)	H5	0.90(5)	
C(6)	C(1)	1.388(10)		N(2)	H6	0.99(5)	
S	O(1)	1.419(6)		C(8)	H7	0.89(5)	
S	O(2)	1.419(6)		C(8)	H8	0.91(5)	
S	N(1)	1.644(6)		C(9)	H9	0.76(5)	
N(1)	C(7)	1.380(9)		C(9)	H10	0.92(5)	
C(7)	O(3)	1.221(8)		C(10)	H11	0.91(5)	
C(7)	N(2)	1.318(9)		C(10)	H12	0.93(5)	
N(2)	C(8)	1.475(10)		C(10)	H13	0.85(5)	
b) Bond angles in (°)							
Cl	C(4)	C(3)	119.1(7)	H1	C(2)	C(1)	124.4(26)
Cl	C(4)	C(5)	119.2(7)	H1	C(2)	C(3)	116.8(27)
S	C(1)	C(2)	119.0(5)	H2	C(3)	C(2)	112.7(25)
S	C(1)	C(6)	120.8(5)	H2	C(3)	C(4)	127.3(25)
C(2)	C(1)	C(6)	120.2(6)	H3	C(5)	C(4)	111.6(25)
C(1)	C(2)	C(3)	118.7(8)	H3	C(5)	C(6)	129.1(25)
C(2)	C(3)	C(4)	119.9(9)	H4	C(6)	C(1)	111.8(26)
C(3)	C(4)	C(5)	121.7(8)	H4	C(6)	C(5)	127.5(26)
C(4)	C(5)	C(6)	118.7(8)	H5	N(1)	S	115.7(31)
C(5)	C(6)	C(1)	120.7(7)	H5	N(1)	C(7)	118.5(31)
C(1)	S	O(1)	108.5(3)	H6	N(2)	C(7)	128.9(28)
C(1)	S	O(2)	107.8(3)	H6	N(2)	C(8)	108.1(27)
C(1)	S	N(1)	106.0(3)	H7	C(8)	N(2)	103.7(31)
N(1)	S	O(1)	104.4(3)	H7	C(8)	C(9)	110.8(31)
O(1)	S	O(2)	119.9(4)	H7	C(8)	H8	103.2(42)
N(1)	S	O(2)	109.5(3)	H8	C(8)	C(9)	114.6(29)
S	N(1)	C(7)	125.7(5)	H8	C(8)	N(2)	110.2(29)
N(1)	C(7)	O(3)	121.3(6)	H9	C(9)	C(8)	114.5(30)
N(1)	C(7)	N(2)	112.6(6)	H9	C(9)	C(10)	113.8(38)
O(3)	C(7)	N(2)	126.1(6)	H9	C(9)	H10	131.7(48)
C(7)	N(2)	C(8)	122.7(7)	H10	C(9)	C(8)	116.2(30)
N(2)	C(8)	C(9)	113.3(7)	H10	C(9)	C(10)	113.3(30)
C(8)	C(9)	C(10)	110.0(7)	H11	C(10)	H12	121.8(43)
H11	C(10)	C(9)	106.5(34)	H12	C(10)	C(9)	112.8(31)
H11	C(10)	H13	82.5(45)	H13	C(10)	C(9)	109.2(35)
H12	C(10)	H13	120.1(46)				

The estimated standard deviations given in parentheses refer to the last decimal positions of respective values.

by Truter²⁸). The bond lengths S-N(1): 1.644, N(1)-C(7): 1.380, C(7)-N(2): 1.318, N(2)-C(8): 1.475, C(8)-C(9): 1.497, C(9)-C(10): 1.504 and C(7)-O(3): 1.221Å are in good

Table V: Least-squares planes in Chlorpropamide.

Atoms in plane	Atoms out of plane	Distance in Å from best plane	Constant
A. Benzene ring			
C(1)		-0.011	A = -0.4610
C(2)		0.009	B = 0.7188
C(3)		-0.005	C = -0.5204
C(4)		0.001	D = -0.2200
C(5)		-0.003	
C(6)		0.008	
	S	-0.014	
	Cl	0.028	
B. Urea group			
N(1)		0.002	A = -0.1027
C(7)		-0.006	B = 0.6769
O(3)		0.002	C = 0.7289
N(2)		0.002	D = 2.7345
	S	0.234	
	C(8)	0.083	
	C(9)	-1.231	
	C(10)	-1.044	

Equation for the plane: $Ax + By + Cz = D$, where x, y, z are in Å.

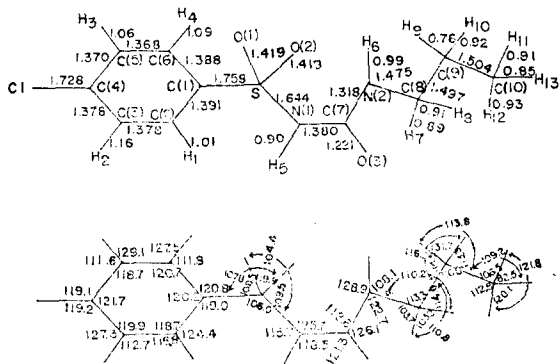


Fig. 1: Bond lengths(Å) and angles (°) with atomic numbering of chlorpropamide.

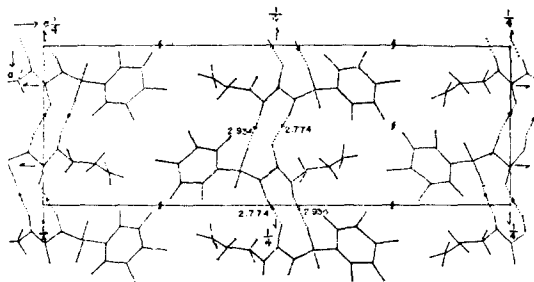


Fig. 2: The crystal structure of chlorpropamide viewed down the b axis.

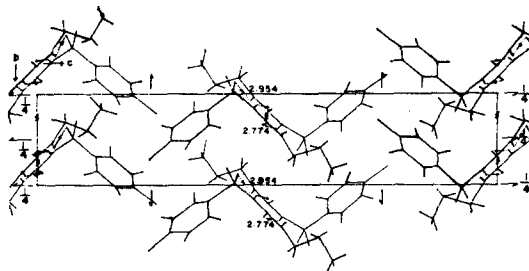


Fig. 3: The crystal structure of chlorpropamide viewed down the a axis.

agreement with the corresponding bond lengths of the related compounds, sulfadiazine¹⁹, sulfaguanidine monohydrate¹⁸, sulfadimethoxine²⁰, sulfisoxazole²², and N'N-bis(3,4-dichlorophenyl) urea²⁷). The C-H and N-H bond lengths are in the range 0.76–1.16Å. The least-squares planes of the benzene ring and the urea group were calculated and the displacements of the atoms from the planes are listed in Table 5. The dihedral angle between the planes through the benzene ring and the urea group is 99°. The conformational angle formed by the projection of the S-C(1) with that of N(1)-C(7) when the projection is taken along the S-N(1) bond is 76°. The molecule appears to form two hydrogen bonds, N(1)-H...O(3) and N(2)-H...O(2)

of length 2.774 and 2.954Å respectively related by screw diads parallel to the a axis. Adjacent molecules parallel to b and c axis are bound together by van der Waals forces.

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