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The Crystal and Molecular Structure of N_1-Cyclohexyl-N_2-(*o*-Chlorobenzal) Imino Thiourea

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Abstract—N_1-Cyclohexyl-N_2-(o-chlorobenzal) imino thiourea, $C_{14}H_{18}N_3SCl$, crystallizes in C_2/c, with $a=19.68$, $b=7.74$, $c=20.42$Å, $\beta=92.8°$ and eight formula units in the unit cell. The structure was solved by the study of Patterson sections, calculated from three-dimensional film data, and was refined by block-diagonal least-squares methods to R=0.16 based on 1288 independent intensity data. The rest atoms of N_1-cyclohexyl-N_2-(o-cholorobenzal) imino thiourea molecule excluding cyclohexan ring and chlorine atoms approximately lie on a plane. A pair of molecules related by the symmetry centers are connected directly with the N-H·····S hydrogen bonds. Apart from the hydrogen bonding system the structure is held together by the van der Waals forces.

A large number of aromatic and heterocyclic thiosemicarbazone derivatives with antibacterial and antitumor activity were reported by French, *et al.*[1~3] Their hypothesis was that a thiosemicarbazone which could function as a tridentate chelate capable of forming octahedral complexes with metal ions would possess antibacterial and antitumor activity. Much later Mathew and Palenik[4] showed, by precision X-ray diffraction studies, the octahedral formulation to be correct for bis(isoquinoline-1-carboxaldehyde thiosemicarbazanato nickel(II) monohydrate. They found the two ligands tridentately bound in two orthogonal planes.

A comparison of the results of Palenik and coworker's[5] structural studies on antitumor active 5-hydroxy-2-formylpyridine thiosemicarbazone sesquihydrate and inactive acetone thiosemicarbazone with the available structural data on other thiosemicarbazones suggested some generalizations regarding the electronic structures, complexing abilities and biological activities of thiosemicarbazones. They suggested that planar mono-negative tridentate nature of thiosemicarbazones appears to be an essential feature for the activities.

Apparently a knowledge of conformation and bond lengths and angles which result from structure analysis could be much meaninigful for the study of biological activity. Therefore,

a crystal structure analysis of N_1-cyclohexyl-N_2(o-chlorobenzal) imino thiourea was undertaken as part of a program devoted to explain the relationship between three dimensional structure of thiosemicarbazone and its biological activities.

EXPERIMENTAL

Suitable evenly developed single crystals were grown by slow evaporation from a solution of *N,N*-dimethyformamide at room temperature. Oscillation and Weissenberg photographs were taken with crystals mounted along the *b* and *c* axes respectively with CuKα radiation.

The unit cell dimensions were determined from the two zero-layer Weissenberg photographs, on which the diffraction lines of aluminium foil were superposed for calibration.

The density of crystal was measured by the floatation method in a mixture of benzene and carbontetrachloride and agrees well with calculated value.

Crystal data:

N_1-Cyclohexyl-N_2(o-chlorobenzal) imino thiourea, $C_{14}H_{18}N_3SCl$. MW=259.8.

monoclinic, $a=19.68\pm0.05$, $b=7.74\pm0.03$, $c=20.42\pm0.05$ Å, $\beta=92.8\pm0.3°$, $V=1691$ Å^3, $D_m=1.26$, $D_x=1.26$ g cm^{-3}, $Z=8$

Systematic absences (hk$l$ for $h+k=2n+1$, h0l for $l=2n+1$ and $h=2n+1$ and 0k0 for $k=2n+1$)

were consistent with space groups Cc and C_2/c. The centric space group was confirmed by the successful solution and refinement of the structure.

For determination of the structure, intensity data were collected with CuKα radiation for layers hk$l$, k=0 to 6 and hk$l$, l=0 and 1, by mounting the crystals about the *b* and *c* axes, respectively with an equi-inclination Weissenberg goniometer, using the multiple film technique. The relative intensities were estimated visually with aid of a set of graded intensities recorded for the same specimen. A total of 1288 independent reflections was observed. The intensities were corrected for the spot-shape, Lorentz and polarization factors. No corrections either for absorption or extinction were made.

The intensities were then scaled to a common base by correlating various layers. An overall scale factor 13.9 and overall temperature factor B=2.45 Å^2 were computed by Wilson's method[6].

STRUCTURE DETERMINATION AND REFINEMENT

A three-dimensional sharpened Patterson synthesis was evaluated, and the prominent peaks on Harker section and line were easily interpreted as Cl-Cl vectors. A structure factor calculation with chlorine contribution alone gave an R index of 0.54. The possible positions for the S atoms could be deduced from a chlorine-phased electron density map on (h0l) calculated with 128 reflections. The R index based on the chlorine and sulfur atoms was 0.49 for the 1044 reflections. A subsequent three-dimensional Fourier synthesis showed the nineteen peaks

which were consistent with a chemically reasonable model for the molecule. At this stage the structure factor calculation for 19 atoms gave a discrepancy index R=0.35, with a uniform isotropic temperature factor, 2.45 Å^2.

Then the structure was refined isotropically using an IBM 1130 block-diagonal least-squares program by Shiono(1968)[7]. The quantity minimized was $\sum w(|F_o|-|F_c|)^2$. The weighting scheme proposed by Cruickshank(1965)[8] was used throughout the refinement. The form of the function, w, was $(a+|F_o|+c|F_o|^2)^{-1}$, where $a=2|F_{min}|=40.10$ and $c=2/|F_{max}|=0.007$ and the refinement was terminated where none of the parameter shifts exceeded one sixth of the corresponding estimated standard deviations. Final R index is 0.16 for all observed reflections.

The positional and thermal parameters for the non-hydrogen atoms together with their estimated standard deviations are listed in Table I. Atomic scattering factor values were taken from the International Table for X-ray crystallography[9]. The observed and calculated structure factors of the observed reflections are listed in Table II.

RESULT AND DISCUSSION

The bond lenths and angles are given in Table III and Fig. 1 where the numbering of the atoms is indicated.

Table I -Final atomic coordinates and isotropic thermal parameters. The estimated standard deviations given in parentheses refer to the last decimal positions

	x	y	z	B(Å)
Cl	0.496(1)	0.014(3)	0.654(1)	2.0(4)
S	0.236(1)	0.617(3)	0.405(1)	3.0(3)
N(1)	0.364(2)	0.614(8)	0.372(2)	2(1)
N(2)	0.351(2)	0.701(8)	0.476(2)	2(1)
N(3)	0.419(2)	0.715(8)	0.485(2)	2(1)
C(1)	0.550(5)	0.936(15)	0.598(5)	8(3)
C(2)	0.617(3)	0.933(9)	0.608(2)	3(1)
C(3)	0.662(3)	0.866(10)	0.564(3)	3(1)
C(4)	0.637(3)	0.762(10)	0.512(3)	3(1)
C(5)	0.563(3)	0.728(10)	0.505(3)	3(1)
C(6)	0.519(3)	0.823(10)	0.546(3)	2(1)
C(7)	0.440(3)	0.797(9)	0.536(3)	2(1)
C(8)	0.324(3)	0.650(10)	0.414(3)	2(1)
C(9)	0.349(3)	0.551(10)	0.305(3)	3(1)
C(10)	0.410(2)	0.461(9)	0.279(2)	2(9)
C(11)	0.394(5)	0.392(15)	0.204(14)	7(2)
C(12)	0.377(4)	0.543(12)	0.163(3)	4(1)
C(13)	0.317(4)	0.643(12)	0.190(3)	4(2)
C(14)	0.327(4)	0.698(13)	0.257(4)	5(2)

Table II-Observed and calculated structure factors. Columns are: Index, F_{obs}, F_{cal}

h=0 k=0

4	39.13	35.03
6	49.77	45.47
8	45.17	36.46
10	67.36	54.11
12	36.74	28.58
16	65.68	50.08
20	46.47	36.65

h=2 k=0

2	119.50	102.69
4	112.97	94.86
6	157.39	143.73
8	64.10	51.20
10	214.26	181.04
12	55.95	43.91
16	36.96	27.77
22	25.98	17.52

h=4 k=0

0	102.49	87.54
2	29.89	32.24
4	171.51	149.82
10	40.84	32.90
14	30.18	33.24
16	54.75	45.39
20	30.93	24.55
24	16.27	11.47

h=6 k=0

0	97.56	86.59
6	62.02	70.66
8	28.79	24.69
12	28.90	19.57
16	39.11	31.28

h=8 k=0

0	123.14	104.04
2	141.42	118.67
4	208.44	191.28
8	81.64	70.63
12	21.43	14.48
16	41.91	33.05
18	17.05	11.99
20	34.61	26.39
22	9.72	6.18

h=10 k=0

0	44.96	38.02
2	51.83	42.52
6	52.65	44.39
8	58.21	47.19
10	72.29	57.76
14	87.67	66.11

h=12 k=0

0	92.62	84.64
4	68.05	55.76
8	34.14	25.73
12	17.01	10.53
20	20.00	14.26

h=14 k=0

0	35.95	29.89
2	68.90	58.00
4	26.60	17.45
8	18.39	12.96
10	56.19	46.58
14	45.22	36.18
18	13.49	12.67

h=16 k=0

0	37.74	28.52
2	18.10	14.28
4	64.65	52.25
8	22.91	17.42
10	23.62	17.14

h=18 k=0

2	26.41	19.12
8	17.58	14.20
10	22.46	17.18
12	20.19	14.41
14	11.62	8.91

h=20 k=0

2	19.23	15.36
4	22.24	18.40
10	15.76	10.66
12	16.82	11.26

h=22 k=0

0	18.42	12.56
2	11.54	7.28

h=24 k=0

2	11.07	6.83
4	13.48	9.68

h=1 k=1

0	50.69	53.08
1	78.07	89.62
3	64.08	67.28
4	82.66	86.61
5	118.83	121.51
7	46.50	38.60
8	44.32	46.98
9	76.82	66.68
10	50.69	45.14
12	65.53	52.83
13	14.12	15.52
14	21.38	20.12
15	22.22	17.92
16	21.15	17.88

h=3 k=1

0	209.26	269.93
1	144.77	148.07
2	184.29	216.98
3	7.18	5.88
4	141.47	151.71
5	46.92	57.35
6	170.02	164.35
7	5.21	5.12
8	59.27	73.18
9	85.13	72.75
11	82.06	69.00
12	36.36	36.76
13	44.11	36.41
14	9.23	4.72
15	37.94	27.99
16	11.47	9.74
17	12.36	10.78
18	12.64	6.50
19	5.09	3.67
20	19.99	16.32
22	14.69	8.91

h=5 k=1

0	161.10	167.14
1	83.01	81.22
3	67.78	59.45
4	22.57	16.26
5	44.37	41.34
6	44.45	53.98
7	28.26	33.92
9	42.85	37.57
10	84.99	72.54
11	28.26	31.29
14	75.73	60.25
15	19.20	15.50
16	51.76	41.18
20	22.62	19.11

h=7 k=1

0	19.46	18.27
2	38.12	29.59
3	26.50	27.38
4	51.66	47.72
5	4.88	4.85
6	59.92	48.09
7	15.71	12.57
8	37.34	29.38
10	56.14	42.32
12	7.54	6.26
13	19.57	14.59
18	19.61	17.16
19	32.02	24.39
20	14.59	12.51
21	22.12	16.70
14	14.95	11.61
24	17.74	13.21

h=9 k=1

0	96.74	86.46
1	59.55	63.05
2	33.88	32.22
3	55.41	45.11
4	71.25	79.13
7	20.16	16.63
9	34.16	30.43
12	52.41	28.01
13	32.11	23.69
18	16.28	12.51

h=11 k=1

1	22.54	19.65
2	60.32	47.38
3	29.50	25.45
4	30.18	30.89
5	26.47	27.80
6	72.23	60.86
7	7.89	7.43
8	49.35	42.23
9	21.57	19.07
10	88.95	74.90
12	41.30	33.27
14	66.61	52.56
15	44.76	34.96
17	13.47	10.47
22	12.19	7.31

h=13 k=1

0	54.83	44.46
2	20.23	16.49
4	44.78	35.40
7	25.28	20.34
8	24.65	21.13
9	75.10	62.83
10	30.46	24.49
11	54.89	44.35
12	25.21	20.71
13	24.13	19.74
14	44.78	34.97
16	23.10	17.36
18	11.48	7.97
19	12.65	9.16
20	10.53	7.61
21	6.30	3.92

h=15 k=1

1	23.81	19.88
6	34.99	26.45
10	16.54	11.25
14	13.11	8.92
20	3.81	2.06

h=17 k=1

1	58.43	46.84
1	11.20	8.52
3	35.64	29.26
4	22.68	20.55
5	29.77	27.77
6	19.40	15.03
11	17.85	12.38
13	12.10	8.60
16	11.89	7.72

h=19 k=1

8	11.31	7.82
11	2.08	1.50
15	3.40	3.11
16	2.59	2.24

h=21 k=1

0	11.43	7.79
1	12.79	10.68
4	27.37	20.02
7	9.21	6.08
13	15.32	10.85

h=23 k=1

1	10.42	7.05
3	5.90	3.19
6	4.41	1.74
7	7.01	4.18

h=0 k=2

0	17.42	26.80
1	155.60	193.76
3	277.59	254.08
4	275.13	249.14
5	73.95	71.74
7	41.02	43.73
8	47.05	40.07
9	35.10	27.12
10	28.81	27.02
11	31.44	22.27
13	71.22	55.27
14	32.39	27.62
15	39.69	30.26
16	32.48	24.30

h=2 k=2

0	68.88	61.20
1	12.89	9.29
2	128.11	111.84
3	48.29	45.56
4	64.90	65.32
5	25.49	20.39
6	43.49	47.71
7	38.00	37.99
8	100.23	84.26
9	111.97	92.30
10	29.86	24.28
12	35.13	29.65
13	39.37	32.13
14	65.67	54.89
18	15.91	11.27
20	19.59	14.10
24	5.01	3.89

h=4 k=2

0	86.55	72.45
1	10.17	11.93
2	37.81	41.79
3	26.45	17.64
4	27.16	33.34
5	45.52	40.86
6	55.12	62.93
7	29.79	29.69
8	75.19	69.11
9	57.49	55.46
10	52.65	42.93
11	46.64	49.79
12	58.69	48.94
17	40.47	38.77
20	13.17	9.67

h=6 k=2

0	36.36	49.27
1	9.69	2.39
3	33.06	33.74
4	72.51	61.82
5	36.38	29.77
6	94.10	75.68
7	58.72	55.48
8	15.77	12.01
9	24.93	19.11
15	31.14	28.23
17	29.77	25.88
19	15.93	11.29

h=8 k=2

0	138.95	116.91
1	100.45	82.92
3	48.92	49.18
4	29.44	32.21
5	69.29	63.48
6	58.18	54.67
7	78.87	64.08
8	28.94	32.83
10	16.59	15.06
11	18.74	12.45
14	25.96	21.12
15	14.12	10.09
16	28.57	22.68
17	17.66	13.04
21	12.19	8.78

h=10 k=2

0	76.42	68.26
1	86.31	78.79

Table II (Cont'd.)

2	24.28	24.56
3	53.86	44.09
5	26.79	26.07
6	55.86	46.86
7	50.05	42.94
8	47.51	38.99
10	42.53	37.14
11	55.68	41.91
13	31.59	23.92
16	19.95	14.11
17	20.67	13.39
22	5.16	3.54

h=12 k=2

1	30.32	31.14
4	77.63	30.97
6	24.42	24.78
7	20.44	22.06
10	76.14	20.51
13	22.36	16.23

h=14 k=2

1	18.49	13.72
5	62.62	49.73
7	28.80	20.92
10	21.71	16.66
13	21.95	24.76
15	17.57	13.72
17	18.55	14.38

h=16 k=2

1	49.34	39.44
8	27.57	25.56
12	15.86	11.42
16	8.06	6.31
17	8.03	6.39

h=18 k=2

1	28.87	21.42
5	17.76	14.06
6	17.20	13.35
12	3.12	1.29

h=20 k=2

0	21.26	17.06
1	6.33	4.98
11	11.65	7.26

h=22 k=2

0	10.18	7.46
1	1.48	0.97
5	5.68	2.81
9	9.60	6.31

h=24 k=2

0	6.54	4.21
1	5.55	4.26
5	10.00	8.19

h=1 k=3

0	76.70	69.58
1	17.01	20.14
4	179.89	118.25
5	98.96	84.92
6	123.67	103.88
7	32.11	23.99
8	57.07	58.22
9	76.51	64.01
10	32.66	29.08
11	14.22	12.43
13	12.05	8.40
14	17.96	20.23
15	2.00	1.64
16	9.81	8.57
22	8.04	6.37
23	8.81	8.30
24	11.33	8.87

h=3 k=3

1	84.11	86.80
2	7.20	5.13
3	12.05	12.26
4	75.91	64.92
6	58.03	49.20
7	26.88	32.58
8	72.49	59.48
9	2.75	2.11
10	39.92	39.89
11	40.61	36.08
12	23.45	24.13
14	41.98	41.26
15	62.35	47.96
16	23.69	18.45
20	13.25	9.25

h=5 k=3

0	56.53	55.32
1	39.10	46.37
2	84.79	82.48
4	57.22	58.26
5	26.88	29.03
6	28.94	25.70
8	33.47	32.55
10	16.57	12.47
11	48.60	42.39
14	20.81	17.95
22	13.79	9.42

h=7 k=3

0	64.12	53.86
1	14.40	17.20
2	27.30	22.33
3	39.24	34.36
4	54.65	45.42
8	45.01	36.83
9	13.71	13.96
10	40.89	43.54
12	24.01	22.09
15	31.00	26.99
16	35.70	26.63
17	16.73	16.38
22	9.84	6.79
23	3.67	3.71

h=9 k=3

1	17.69	12.55
2	33.98	26.13
6	64.76	55.93
9	67.64	52.64
10	43.28	33.02
12	23.32	18.89
14	17.01	14.78
21	7.03	4.81
22	7.81	6.17

h=11 k=3

0	85.69	69.53
2	13.58	14.34
3	71.66	58.30
4	14.96	12.51
5	16.73	17.57
6	22.75	21.43
7	31.82	33.76
9	58.95	48.89
10	18.63	15.59
11	42.97	33.00
12	37.62	27.35
16	21.62	16.73
18	19.20	13.98
19	21.53	15.26
21	10.84	7.93

h=13 k=3

2	15.23	17.56
3	23.60	29.03
5	50.82	42.07
6	63.12	50.60
7	24.60	22.68
8	56.05	45.35
9	5.69	2.90
10	24.01	25.01
13	29.32	23.26
15	27.22	20.75
16	8.22	5.87
17	14.70	11.34

h=15 k=3

0	35.53	32.25
1	26.88	28.37
2	23.45	23.32
4	25.66	20.95
7	15.57	12.33
16	13.87	10.89

h=17 k=3

2	23.85	18.51
7	31.69	26.46
9	27.47	18.63
10	12.58	9.00
14	11.57	7.89

h=19 k=3

3	16.95	14.06
8	19.14	15.25
13	13.85	10.47

h=21 k=3

2	10.95	8.17
3	10.80	6.60
6	10.44	8.54
8	3.32	1.71
9	12.82	10.30
10	13.08	8.76

h=23 k=3

0	15.76	11.70
1	11.50	9.20
3	8.85	6.06
4	15.75	10.15

h=0 k=4

1	13.99	15.81
4	91.48	74.58
5	85.75	70.51
6	157.01	132.13
7	70.41	58.63
7	53.54	46.38
9	64.15	51.62
10	70.98	54.41
12	14.57	10.86
14	18.52	21.89
18	14.57	11.37
22	17.92	13.55

h=2 k=4

0	111.00	136.80
1	17.42	21.84
2	41.25	38.96
3	64.82	57.09
4	28.69	28.74
5	33.16	29.17
6	37.46	42.68
7	47.74	43.61
9	8.33	6.97
10	7.24	7.49
11	12.54	9.31
12	6.62	2.41
13	13.85	13.00
16	44.71	33.61
19	14.15	11.43
21	7.74	4.67

h=4 k=4

0	3.19	3.01
1	10.69	12.14
2	40.89	43.50
4	54.22	45.48
5	16.36	14.81
6	39.92	41.84
9	5.61	4.09
10	77.66	69.66
13	25.41	23.22
14	36.28	30.34
20	15.28	10.46

h=6 k=4

0	42.45	33.52
2	57.20	44.69
3	15.01	8.85
4	57.49	58.68
6	30.87	26.36
7	29.09	29.31
8	17.83	19.19
9	14.26	14.60
11	19.34	23.42
16	35.56	29.17
19	5.05	3.36
10	28.83	21.00

h=8 k=4

1	15.08	16.33
2	24.01	22.62
3	19.89	15.25
5	5.32	2.23
6	35.25	33.03
8	43.96	38.22
10	39.18	30.48
12	13.17	8.09
13	9.30	7.50
14	24.36	17.56

h=10 k=4

0	39.92	37.36
1	26.34	32.37
2	6.85	5.72
4	111.66	91.93
7	3.86	3.98
8	45.01	43.61
9	43.87	33.96
13	14.14	11.83
16	17.88	12.33
18	11.37	6.44
20	7.80	4.66

h=12 k=4

0	13.30	11.86
1	27.85	27.23
7	12.83	9.94
9	8.18	7.02
10	31.41	25.20
14	38.94	29.31

h=14 k=4

0	58.72	46.21
1	23.87	19.40
2	16.87	14.65
3	39.29	31.14
4	19.52	13.37

h=16 k=4

0	9.07	8.39
2	24.55	27.02
10	15.91	15.36
13	8.92	7.81
14	10.16	7.66
15	6.96	4.50

h=18 k=4

2	14.77	11.92
4	30.59	26.17
8	19.14	14.96
12	13.40	9.36

h=20 k=4

2	12.68	8.60
10	10.24	8.05

h=22 k=4

2	6.22	2.73
5	10.82	7.44

h=1 k=5

0	27.98	25.52
1	12.48	27.28
4	39.78	48.63
5	30.34	31.03
6	82.47	76.60
7	19.53	19.56
9	18.32	16.81
10	25.17	21.26
11	28.40	23.61
13	26.20	24.24
15	18.31	13.88
19	10.52	7.25
20	16.19	13.71
21	21.46	0.92

h=3 k=5

0	53.20	53.22

Table II (Cont'd.)

2	46.10	53.22
3	20.95	15.25
4	34.50	29.35
5	32.87	25.63
6	27.68	20.26
7	10.42	13.34
8	38.15	31.34
10	39.94	33.28
12	47.62	37.22
13	4.19	2.64
14	19.20	18.28
16	13.58	12.51
18	14.67	12.52
21	1.16	0.96

h=5 k=5

0	27.39	22.99
1	2.41	1.26
3	31.00	27.53
6	36.25	27.41
10	14.12	11.80
17	9.29	6.69
18	12.21	8.71
19	6.62	5.18
20	6.60	4.01

h=7 k=5

0	59.27	52.47
1	44.04	37.69
2	28.67	34.86
3	24.55	23.53
4	20.30	19.43
11	9.90	6.52
12	22.08	18.41
13	28.57	23.75
14	34.11	26.56
16	13.02	13.16

h=9 k=5

0	32.53	29.01
2	39.51	36.48
3	21.13	17.22
6	24.87	22.87
7	26.26	19.53
8	14.81	13.88
10	31.14	29.78
15	16.59	9.24
19	5.56	2.66
20	12.34	7.07

h=11 k=5

0	34.43	31.84
1	14.12	11.18
3	12.48	14.41
4	49.26	41.47
6	28.40	27.63
8	38.39	29.61
9	36.01	26.48
12	15.49	15.41

h=13 k=5

1	31.69	31.42
2	17.18	12.95
3	33.43	26.55
4	49.02	39.53
10	13.30	11.96
11	7.39	6.19
17	9.87	4.68

h=15 k=5

0	35.25	31.08
1	13.63	11.52
4	22.22	19.71
8	13.02	12.29
13	6.76	4.60
14	6.60	6.16

h=17 k=5

6	19.49	13.70
10	21.42	14.97

h=19 k=5

0	13.37	8.87

h=0 k=6

3	35.61	34.75
4	8.48	6.16
5	26.48	20.86
6	18.80	13.84
7	48.98	37.22
8	21.24	15.77
9	30.87	29.00
10	51.17	46.59
15	7.54	5.39

h=2 k=6

0	19.58	20.26
3	54.21	50.31
4	25.32	19.88
5	39.48	32.58
7	10.28	8.83
8	2.71	2.87
9	15.23	13.02
10	16.18	18.79

h=4 k=6

0	35.12	38.53
1	40.74	33.62
6	22.88	19.10
7	13.99	15.94
9	3.10	1.70
13	20.85	17.68
17	10.62	7.94
18	19.07	0.48

h=6 k=6

0	62.23	50.13
3	32.01	24.32
4	20.74	18.34
7	28.05	26.49
11	7.63	4.95

h=8 k=6

1	23.13	22.88
3	14.81	25.17
5	32.93	31.64
6	12.51	9.89
8	7.69	6.71
9	12.52	9.62

h=10 k=6

0	24.83	27.41
7	34.16	28.80
16	3.39	2.32

h=12 k=6

0	25.24	19.87

h=14 k=6

1	20.71	18.82
7	9.36	7.01

h=16 k=6

5	22.91	19.05

h=2 k=0

−2	184.70	160.00
−4	202.01	170.62
−6	190.60	216.37
−10	24.83	25.29
−14	60.23	49.43
−18	63.74	48.91

h=4 k=0

−2	27.20	23.95
−4	173.03	184.40
−6	113.10	100.80
−8	89.37	75.77
−10	55.18	49.00
−12	124.83	106.95
−16	78.28	63.14
−20	40.27	29.57

h=6 k=0

−2	144.90	150.61
−4	70.18	56.04
−6	103.98	89.21
−8	62.30	51.52
−10	158.48	168.55
−12	45.36	36.16
−14	12.48	17.86
−20	13.17	9.86
−22	19.98	13.66

h=8 k=0

−2	76.95	64.16
−4	97.22	83.75
−8	20.61	14.78
−10	45.36	39.41
−12	32.59	20.90
−16	36.69	31.05

h=10 k=0

−2	159.67	131.00
−4	36.24	34.38
−6	57.22	52.67
−8	21.22	14.85
−18	26.57	19.07
−22	23.17	18.12

h=12 k=0

−4	95.09	89.90
−6	16.32	10.89
−8	60.75	52.51
−10	33.75	30.77
−12	26.93	20.21
−14	42.14	30.84
−16	52.99	41.43
−18	30.36	22.89

h=14 k=0

−2	6.50	4.53
−6	174.23	139.39
−8	88.33	72.94
−12	20.73	15.47
−22	9.27	4.79

h=16 k=0

−2	54.58	43.31
−14	17.98	13.18
−18	16.66	11.71

h=20 k=0

−4	8.85	5.94
−8	34.86	26.95
−10	19.27	14.36
−16	20.01	15.56

h=22 k=0

−2	22.59	16.80
−4	21.11	15.22
−8	15.22	10.67

h=24 k=0

−8	5.36	3.19

h=1 k=1

−3	48.57	48.48
−4	177.98	180.36
−6	23.18	22.48
−7	24.01	24.75
−8	82.46	70.54
−9	15.91	9.40
−10	88.15	75.80
−12	20.21	18.16
−13	20.96	17.62
−14	33.34	24.80
−15	52.88	45.11
−16	47.49	39.45
−17	70.18	56.98
−18	23.22	20.02
−18	22.96	19.22
−20	46.14	35.46
−24	16.89	12.51

h=3 k=1

−1	46.59	39.95
−5	152.45	146.27
−6	66.68	58.00
−7	54.33	55.32
−8	84.38	79.88
−10	103.74	87.77
−11	57.93	49.99
−12	48.08	39.30
−13	28.73	29.30
−14	58.00	48.55
−16	32.28	26.43
−18	56.36	44.88
−19	41.14	32.73
−20	13.39	10.85
−21	30.26	30.17
−23	13.96	10.48

h=5 k=1

−1	17.85	14.58
−2	107.72	93.79
−3	88.37	84.58
−4	83.43	82.33
−5	29.52	22.86
−6	79.72	79.20
−7	13.30	14.69
−8	24.36	17.90
−9	17.83	19.09
−10	29.27	24.22
−11	41.50	33.48
−12	4.17	0.73
−15	18.35	13.71
−16	35.63	27.19
−18	23.56	15.49
−19	8.75	6.65

h=7 k=1

−1	108.81	100.59
−4	69.96	59.04
−5	36.41	33.26
−6	48.43	51.06
−7	54.60	55.07
−8	47.20	43.85
−9	10.22	5.20
−10	77.12	66.49
−11	39.65	35.20
−12	34.81	26.04
−14	44.14	35.05
−16	23.18	16.92
−18	14.99	11.93

h=9 k=1

−1	31.14	36.68
−2	46.31	50.41
−3	58.86	61.02
−4	39.41	32.03
−6	48.16	45.90
−7	36.85	26.61
−8	17.14	23.28
−11	29.91	27.91
−12	21.95	9.95
−16	35.80	28.94
−19	18.93	13.61
−20	30.73	23.48

h=11 k=1

−1	80.93	66.37
−2	16.59	15.26
−3	55.24	45.16
−5	23.32	22.34
−6	102.38	94.53
−7	19.77	15.69
−8	13.88	8.04
−9	21.10	16.09
−10	75.26	61.41
−12	27.30	22.09
−13	31.97	26.03
−15	17.63	13.97
−16	10.55	6.84
−17	14.11	10.60
−19	16.68	12.10
−22	8.08	4.80

h=13 k=1

−1	19.02	14.33
−3	34.84	31.24
−4	53.08	42.58
−6	19.75	21.93
−7	20.78	16.13
−11	23.31	17.63
−12	30.35	23.17
−13	32.60	23.74
−14	24.53	18.73
−16	18.95	14.59

h=15 k=1

−1	19.83	13.49
−2	66.68	55.56
−3	26.34	29.07

Table II (Cont'd.)

−4	59.83	47.08
−5	34.13	28.08
−6	38.14	35.09
−7	42.05	33.52
− 9	41.37	33.71
−10	36.02	26.90
−14	14.90	10.43
h=17 k=1		
−2	24.96	19.73
−3	26.90	22.17
−4	37.07	30.85
−11	21.37	15.89
−13	20.65	15.88
−16	27.26	20.97
h=19 k=1		
−3	9.66	6.96
−10	18.19	14.38
h=21 k=1		
−7	17.18	12.40
−9	7.94	6.14
−12	16.48	12.29
h=23 k=1		
−3	13.86	10.45
−5	15.13	11.15
−6	22.41	17.17
h=2 k=2		
−2	113.21	102.40
−3	41.02	38.55
−4	147.70	126.47
−5	41.60	35.05
−7	74.23	70.81
−8	52.96	58.77
−9	34.90	36.77
−10	70.39	66.77
−11	16.59	18.26
−12	24.17	18.13
−13	16.32	21.20
−14	18.89	15.73
−15	46.51	37.59
−16	46.37	36.70
−19	22.91	17.80
−22	16.26	12.26
−24	9.76	6.91
h=4 k=2		
−2	65.17	65.86
−3	47.05	64.49
−4	44.25	38.31
−5	72.64	62.22
−6	92.40	78.69
−7	46.27	36.69
−9	108.54	92.95
−10	17.96	19.44
−11	20.98	25.43
−12	43.95	38.24
−13	50.22	46.47
−14	32.91	26.68
−15	21.13	25.28
−16	42.25	34.66
−17	26.26	19.13
−18	13.66	10.61
−19	38.40	28.97
−22	14.04	10.14
−23	16.72	11.48
h=6 k=2		
−1	107.30	109.73
−3	111.97	96.21
−4	37.95	31.40
−5	51.94	43.25
−6	149.12	125.04
−7	65.17	63.51
−8	45.35	38.43
−9	42.12	41.34
−12	37.82	30.93
−13	85.56	69.96
−14	42.42	35.68
−20	14.47	10.13
−22	11.07	8.07
−23	9.86	6.74
−24	2.82	2.62
h=8 k=2		
−1	90.63	76.07
−2	26.30	23.81
−3	68.08	56.12
−4	48.61	41.63
−5	27.57	27.92
−6	60.05	51.89
−10	51.83	41.97
−12	51.48	39.53
−21	19.20	15.54
h=10 k=2		
−1	42.36	45.20
−3	26.75	23.02
−4	29.15	22.92
−5	64.34	50.65
−6	32.75	37.08
−9	19.20	22.17
−10	22.22	20.30
−11	17.96	14.44
−12	25.91	21.27
−13	21.81	20.02
−15	40.58	32.37
−16	19.18	14.62
−18	21.67	17.40
h=12 k=2		
−2	41.98	39.82
−5	83.45	68.06
−6	19.34	22.16
−7	26.20	30.88
−9	24.47	25.93
−11	25.95	21.34
−14	35.05	28.07
−15	27.91	19.77
−17	22.85	15.96
−19	19.20	14.85
−20	14.73	12.00
h=14 k=2		
−2	75.68	61.10
−3	40.67	31.34
−4	70.95	57.67
−5	70.10	56.80
−8	33.94	26.56
−9	65.23	51.18
−10	44.83	37.15
−11	48.64	39.07
−15	18.40	13.97
−19	9.48	5.31
−20	10.23	7.27
h=16 k=2		
−1	17.24	14.99
−4	45.60	35.54
−7	17.93	13.64
−8	20.00	14.55
−10	37.16	29.41
h=18 k=2		
−11	18.68	14.22
−15	9.02	6.21
−18	4.54	3.02
h=20 k=2		
−1	21.59	17.17
−7	22.39	16.28
−12	17.16	12.84
−14	7.74	5.92
h=22 k=2		
−5	20.24	15.25
−12	7.17	5.45
h=24 k=2		
−3	4.28	3.18
h=1 k=3		
−3	24.83	20.71
−4	19.20	20.41
−6	21.20	19.86
−7	60.34	45.09
−8	41.45	35.96
−11	74.32	61.62
−12	56.62	45.46
−13	25.80	23.88
−14	72.89	59.69
−15	19.35	15.42
−16	14.20	12.06
−17	25.92	24.94
−18	21.34	16.21
−21	21.72	17.46
−22	13.44	10.66
−23	14.14	10.13
h=3 k=3		
−1	83.17	68.87
−2	70.79	60.78
−4	95.76	81.51
−5	35.25	41.39
−6	72.00	62.00
−7	40.47	35.90
−8	77.19	63.98
−9	39.59	30.83
−10	1.73	0.55
−11	13.17	13.66
−12	39.69	30.64
−14	22.08	23.20
−15	62.51	50.35
−17	46.93	36.99
−18	32.74	24.80
−20	26.58	15.27
−22	30.18	11.26
−24	14.11	9.70
h=5 k=3		
−1	25.29	20.56
−2	73.87	62.81
−3	39.10	35.13
−4	14.67	14.76
−5	44.45	38.61
−6	71.50	60.87
−7	41.15	42.99
−8	38.96	30.97
−10	71.83	59.33
−12	66.68	53.99
−13	30.88	22.48
−15	31.56	23.41
−16	10.62	7.63
h=7 k=3		
−1	107.58	91.23
−2	85.67	74.67
−3	10.75	9.22
−4	68.44	59.44
−5	61.83	51.95
−6	27.91	24.14
−7	42.24	42.77
−8	19.20	22.76
−11	27.98	34.12
−15	11.09	10.81
−16	31.00	25.65
−17	9.74	8.61
−21	17.45	12.18
−22	10.87	7.72
−23	12.37	8.83
−24	6.43	5.31
h=9 k=3		
−1	65.45	57.64
−2	2.53	2.32
−4	54.50	48.07
−5	14.15	6.94
−6	28.67	26.83
−7	9.60	6.41
−8	26.61	33.23
−9	11.91	10.68
−11	34.84	36.62
−14	25.23	20.05
−19	17.83	15.91
−22	15.15	11.29
h=11 k=3		
−2	34.47	29.66
−3	13.58	14.59
−4	51.60	41.85
−5	28.62	21.65
−7	30.38	23.45
−8	15.23	18.49
−9	23.87	19.61
−11	14.50	11.77
−12	26.05	21.73
−13	35.23	27.97
−14	16.48	13.16
−16	16.56	12.64
−17	18.65	15.13
−19	10.79	7.05
−20	22.35	15.96
−21	9.61	6.49
h=13 k=3		
−3	17.13	13.75
−4	15.36	14.40
−6	38.62	29.95
−7	34.84	29.50
−8	1.29	0.00
−10	53.85	40.13
−12	18.38	14.39
−14	23.60	21.82
−17	17.57	12.64
h=15 k=3		
−1	41.99	33.71
−2	13.43	14.82
−3	41.71	38.79
−4	35.94	37.04
−12	23.45	19.76
−13	22.81	15.18
−15	11.32	7.52
−18	22.52	9.24
−19	8.42	6.03
−20	8.50	5.76
h=17 k=3		
−1	29.72	23.35
−2	25.99	20.11
−3	27.71	23.88
−5	19.61	18.52
−7	23.37	18.92
−9	13.85	10.27
−10	14.46	11.61
−14	9.77	6.35
h=19 k=3		
−4	16.55	12.82
−9	6.83	4.33
−12	12.75	9.77
−13	6.97	5.49
−15	6.26	5.02
h=21 k=3		
−2	14.37	10.37
−5	21.28	15.94
−6	16.66	11.39
−7	13.56	8.60
h=2 k=4		
−3	25.22	23.98
−4	100.30	90.58
−5	21.16	18.17
−6	66.60	55.44
−7	19.15	16.90
−9	24.18	18.33
−10	21.95	20.73
−12	73.37	70.84
−13	42.68	33.13
−15	19.88	16.38
−16	20.45	14.80
−20	24.27	18.17
−22	15.22	9.92
h=4 k=4		
−1	47.36	37.32
−2	71.07	67.72
−3	32.93	34.64
−4	25.51	27.39
−5	77.20	61.06
−6	68.71	58.27
−9	11.11	14.16
−10	66.71	55.43
−12	45.69	41.47
−14	30.87	24.58
−15	35.40	28.12

Table II (Cont'd.)

−16	21.26	21.48
−17	10.07	7.28
−22	19.84	13.46
h=6 k=4		
−1	26.07	18.70
−2	8.17	8.70
−3	55.28	44.47
−4	69.47	59.39
−5	26.16	22.91
−6	41.11	32.35
−7	3.21	0.62
−10	4.29	1.77
−11	22.14	17.10
−12	29.59	22.14
−13	23.46	23.24
−16	48.27	37.74
h=8 k=4		
−1	21.48	15.11
−2	102.99	86.20
−3	29.17	23.42
−4	39.53	33.31
−6	44.04	42.88
−9	13.06	7.14
−10	41.05	32.21
−12	15.46	13.22
−18	13.60	10.07
−22	12.94	10.03
h=10 k=4		
−1	30.09	24.34
−3	11.41	6.97
−4	18.52	18.73
−5	22.65	17.33
−8	28.62	23.28
−10	29.91	34.22
−12	33.81	25.08
−16	24.55	19.66
−19	12.34	11.18
h=12 k=4		
−1	22.70	17.12
−2	41.38	30.71
−4	28.40	34.92
−6	53.51	42.31
−8	31.48	24.40
−9	20.85	19.77
−12	17.42	13.49
−14	17.01	16.94
h=14 k=4		
−1	39.34	30.90
−2	33.63	25.56
−8	29.96	28.15
−10	17.28	15.55
−12	39.52	31.69
−14	21.62	15.79
−15	21.80	16.13
−16	12.33	7.23
h=16 k=4		
−1	17.54	14.21
−3	16.39	12.75
−5	12.82	10.16
−6	36.96	28.34
h=18 k=4		
−10	21.68	15.93
−11	12.08	8.31
−12	14.89	10.38
h=20 k=4		
−2	18.62	14.48
−4	17.93	13.25
−8	11.59	7.56
h=22 k=4		
−4	6.91	4.55
h=1 k=5		
−4	14.40	15.46
−5	52.67	40.87
−7	37.73	37.29
−8	45.95	35.73
−9	44.41	36.41
−10	65.45	51.98
−12	11.47	10.19
−14	22.14	21.67
h=3 k=5		
−1	8.75	10.15
−2	44.65	42.88
−4	32.65	32.58
−6	2.28	3.74
−8	27.73	25.77
−9	21.95	24.06
−10	51.68	41.10
−12	20.00	19.57
−13	10.59	8.09
−14	37.39	28.28
−15	13.38	10.11
−16	26.60	20.43
−17	10.83	10.36
−18	14.81	17.73
−20	11.82	8.52
h=5 k=5		
−1	19.61	22.29
−2	15.12	14.87
−6	57.52	49.13
−7	29.35	32.41
−8	21.95	23.87
−9	20.21	13.80
−10	41.84	39.54
−12	17.94	16.32
−13	9.38	7.68
−14	16.08	13.75
−16	15.64	14.59
h=7 k=5		
−2	30.00	24.48
−4	54.19	56.82
−5	7.80	4.86
−7	31.00	33.64
−6	31.28	33.76
−8	17.55	30.52
−19	9.72	7.66
−20	22.25	16.11
h=9 k=5		
−1	23.60	24.05
−3	10.83	8.71
−4	14.26	15.38
−5	11.38	10.90
−6	33.62	25.74
−7	18.50	13.47
−10	15.68	12.54
h=11 k=5		
−4	14.40	14.69
−6	12.89	14.39
−8	10.83	7.34
−9	24.02	18.61
−10	25.18	19.23
−12	15.79	11.76
−16	28.89	21.37
−18	10.18	7.68
h=13 k=5		
−1	10.83	8.65
−2	17.95	18.97
−6	22.08	19.36
−7	16.33	10.37
−10	28.26	28.33
h=15 k=5		
−4	20.69	19.84
−11	12.27	8.86
−14	15.92	10.95
−16	17.53	12.30
h=17 k=5		
−4	25.73	14.03
−6	25.38	22.53
−10	13.22	9.99
h=21 k=5		
−1	5.75	3.85
h=23 k=5		
−2	18.02	12.97
h=2 k=6		
−2	15.64	14.79
−3	29.52	27.96
−4	21.43	23.87
−9	25.92	29.06
−10	35.06	28.51
−13	20.71	22.74
h=4 k=6		
−1	20.98	18.92
−2	16.26	10.10
−3	26.87	26.85
−4	24.14	22.21
−5	24.70	18.49
−6	41.98	39.38
−8	13.79	11.15
−13	27.44	32.63
−15	24.69	17.98
h=6 k=6		
−3	24.93	22.72
−5	28.79	25.01
h=8 k=6		
−5	32.00	29.71
−6	24.28	23.57
−17	5.53	3.70
h=10 k=6		
−1	20.98	16.64
−5	20.68	20.53
−6	20.14	19.53
−9	14.67	12.08
h=12 k=6		
−9	20.71	21.47
−11	24.55	20.32
h=14 k=6		
−1	25.51	19.41
−13	13.31	9.40
−15	11.78	8.51
h=16 k=6		
−2	16.44	12.11

The ring C-C bond lengths in benzene ring vary from 1.33 to 1.47 Å with the average value of 1.41 Å, which is in agreement with the standard C-C bond length in the benzene ring within the experimental error. It might be pointed out that the internal valence angles (range 117-124°) at the substituted benzene ring generally show significant deviation from the ideal hexagonal value of 120°.

The distance of C-Cl, 1.71 Å is in agreement with the carbon-chlorine distances found in other benzene derivatives such as Tanaka (1974)[10], Holden & Dickinson (1967)[11], Silverman, *et al.* (1971)[12] and Rudman (1971)[13].

The bond length of C-S 1.75 Å is appreciably longer than the pure carbon to sulfur double bond. Namely this length is between the double bond 1.56 Å and the single bond 1.82 Å (Sutton (1965)[14]). Also the length of the C(8)-N(1) bond 1.24 Å is shorter than normal C-N single bond and C(7)-N(3) dislance of 1.28 Å is longer than normal C-N double bond distance. These features can be qualitatively accounted by the contributions of the cannonical

Table III-Bond lengths and angles in N_1-cyclohexyl-N_2-(o-chlorobenzal) imino thiourea. Estimated standard deviations refer to the last decimal positions of respective values

i	j	D_{ij}	i	j	k	∠ijk
C(1)	C(2)	1.33(2)Å	C(2)	C(1)	Cl	123(5)°
C(1)	C(6)	1.41(2)	C(2)	C(1)	C(6)	117(3)
C(1)	Cl	1.71(1)	C(6)	C(1)	Cl	118(5)
C(2)	C(3)	1.40(2)	C(1)	C(2)	C(3)	124(3)
C(3)	C(4)	1.40(2)	C(2)	C(3)	C(4)	119(3)
C(4)	C(5)	1.47(2)	C(3)	C(4)	C(5)	119(3)
C(5)	C(6)	1.43(2)	C(4)	C(5)	C(6)	117(3)
C(6)	C(7)	1.57(2)	C(1)	C(6)	C(5)	120(3)
C(7)	N(3)	1.28(3)	C(1)	C(6)	C(7)	121(3)
C(8)	N(1)	1.24(2)	C(5)	C(6)	C(7)	119(3)
C(8)	N(2)	1.40(2)	C(6)	C(7)	N(3)	116(2)
C(8)	S	1.75(1)	N(1)	C(8)	N(2)	118(2)
C(9)	C(10)	1.51(2)	N(1)	C(8)	S	124(3)
C(9)	C(14)	1.55(2)	N(2)	C(8)	S	118(4)
C(9)	N(1)	1.46(2)	C(10)	C(9)	N(1)	110(2)
C(10)	C(11)	1.61(2)	C(14)	C(9)	N(1)	113(3)
C(11)	C(12)	1.49(2)	C(8)	N(1)	C(9)	128(2)
C(12)	C(13)	1.54(2)	C(8)	N(2)	N(3)	119(2)
C(13)	C(14)	1.44(2)	C(7)	N(3)	N(2)	116(3)
N(2)	N(3)	1.35(3)				

forms which was also found in Restivo and Palenik (1970)[15]. These tendency can be found also in Conde *et al.* (1972)[16]. The planarity around the C(8) which indicates sp^2 hybridization in that atom, suggests a good evidence for this fact.

The least-squares planes are listed in Table IV. The benzene ring is planar within the error of the determination. And two substituted atoms, chlorine and C(7), are displaced −0.15 and −0.01 Å respectively. A little deviation of the heavy atom from the benzene ring can be found in other compound as in Braiss and Jurgen Sygusch (1974)[17].

N_1-Cyclohexyl-N_2-(o-chlorobenzal) imino thiourea is antitumor and antimicrobial agent[18]. It has been pointed out by several investigators[2] that antitumor and antimicrobial activities of thiosemicarbazones are due to their ability to from complexes with metal ions. Gus J. Palenik and coworker[5] suggested that planar mono-negative tridentate nature of the active thiosemicarbazones appears to be an essential feature for the activities. The extensive delocalization involving the thiosemicarbazide side chain and the benzene ring might be a possible explanation for the activities of N_1-cyclohexyl-N_2-(o-chlorobenzal) imino thiourea.

The distances from C(9) and C(12) to the plane contained C(10), C(11), C(13) and C(14) are −0.67 and 0.67 Å respectively, thus the cyclohexane ring has the normal chair confor-

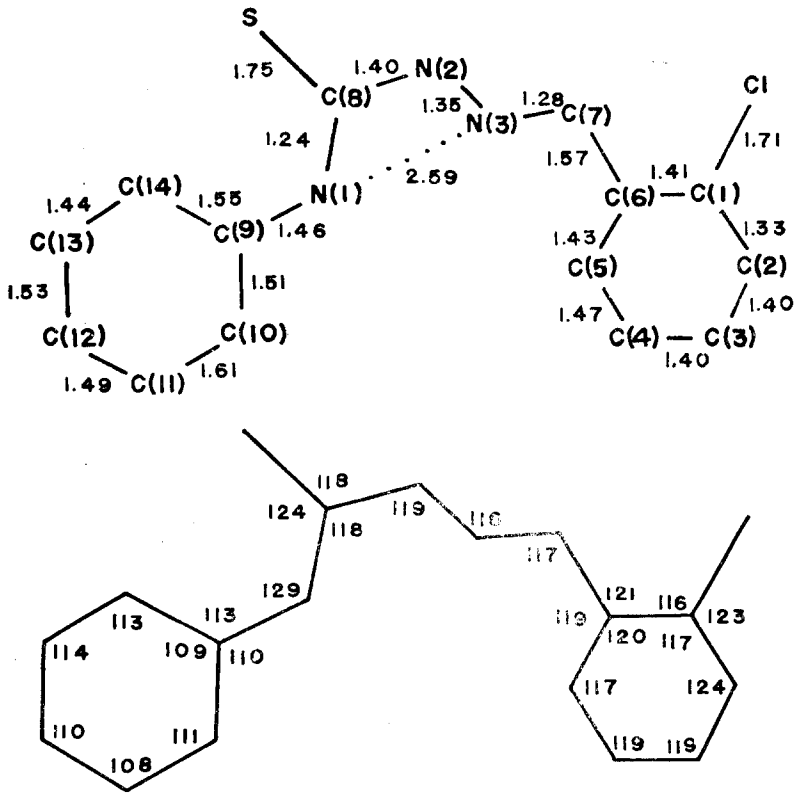

Fig. 1—Bond lengths (Å) and angles (°) in N_1-cyclohexyl-N_2-(o-chlorobenzal) imino thiourea.

mation.

The crystal structure is illustrated in Fig. 2 and Fig. 3 viewed down the *a* and *b* axes respectively.

A pair of molecules related by the symmetry centers are connected directly with the N-H ……S hysdrogen bonds. The length of this intermolecular hydrogen bond is 3.34 Å and the hydrogen bonding scheme is shown as the dotted lines in Fig. 3. Though the positions of hydrogen atoms cannot be located under the present accuracy, it is reasonable to conclude the N-H……N intramolecular hydrogen bond as in D.V. Naik and G.J. Palenik (1974)[19]. The distance from N(1) to N(3) is 2.59 Å.

Apart from the hydrogen bonding system the structure is held together by the van der

Table IV-Least-squares planes in N_1-cyclohexyl-N_2-(o-chlorobenzal) imino thiourea.
Equation for plane: Ax+By+Cz=D, where x,y,z are in Å.

Atoms in plane	Atoms out of plane	Distance in Å from best plane	Constant
A. Benzene ring			
C(1)		0.06	A=−0.09
C(2)		−0.09	B= 0.79
C(3)		0.04	C=−0.61
C(4)		0.04	D=−0.71
C(5)		−0.07	
C(6)		0.02	
	C(7)	−0.01	
	C(8)	0.61	
	Cl	−0.15	
B. Cyclohexane ring			
C(10)		0.02	A= 0.77
C(11)		−0.02	B= 0.57
C(13)		0.03	C=−0.33
C(14)		−0.03	D= 6.31
	C(9)	−0.67	
	C(12)	0.67	
C. Thiosemicarbazide side chain and benzene ring			
N(1)		0.29	A= 0.01
N(2)		−0.17	B= 0.87
N(3)		−0.16	C=−0.49
C(1)		0.22	D= 0.20
C(2)		0.11	
C(3)		0.10	
C(4)		−0.09	
C(5)		−0.26	
C(6)		−0.03	
C(7)		−0.11	
C(8)		0.10	
	S	−0.05	

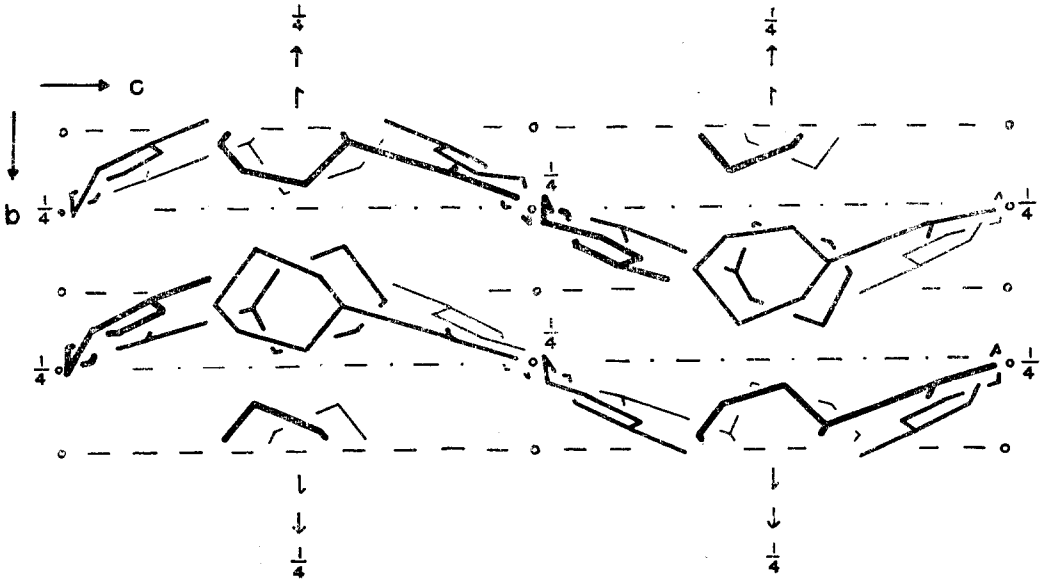

Fig. 2—The crystal structure on N_1-cyclohexyl-N_2-(o-chlorobenzal) imino thiourea viewed down the *a* axis.

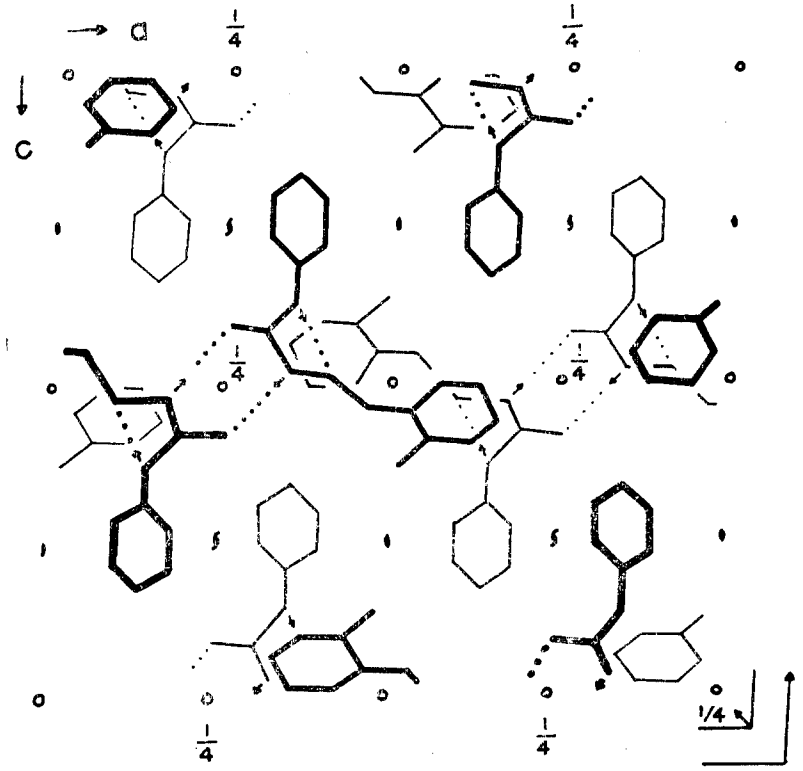

Fig. 3—The crystal structure of N_1-cylohexyl-N_2-(o-chlorobenzal) imino thiourea viewed down the *b* axis. Dotted lines indicate hydrogen bonds with arrows pointing in the donor direction.

Waals forces.

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