ANSELL, G. B. & KATZ, L. (1966). *Acta Cryst.* **21**, 482.
CANNERI, G. (1925). *Gazz. Chim. Ital.* **55**, 611.
COTTON, F. A. & WOOD, J. S. (1964). *Inorg. Chem.* **3**, 245.
DOYLE, P. A. & TURNER, P. S. (1968). *Acta Cryst.* A**24**, 390.
FURNAS, T. C. (1957). *Single Crystal Orienter Instruction Manual.* Milwaukee: General Electric Company.
HAAS, D. J., HARRIS, D. R. & MILLS, H. H. (1965). *Acta Cryst.* **19**, 676.
HOUSTY, J. & CLASTRE, J. (1957). *Acta Cryst.* **10**, 695.
MONTGOMERY, H., CHASTAIN, R. V., NATT, J. J., WITKOWSKA, A. M. & LINGAFELTER, E. C. (1967). *Acta Cryst.* **22**, 775.
STEWART, J. M. (1964). *Crystal Structure Calculations System X-ray-63*, Univ. of Maryland TR-64-6.
STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175.

Acta Cryst. (1970). B**26**, 341

Investigations of Dithienylglycollic Esters. II. The Crystal and Molecular Structure of Quinuclidinyl Di-α,α′-thienylglycollate

BY ANITA MEYERHÖFFER

Department of Medical Physics, Karolinska Institutet, S-104 01 *Stockholm and The Research Institute of National Defence,* S-172 04 *Sundbyberg, Sweden*

(*Received* 9 *April* 1969)

Crystals of quinuclidinyl di-α,α′-thienylglycollate are monoclinic, space group $P2_1$ with two formula units in a cell having the dimensions $a=9{\cdot}762$, $b=11{\cdot}348$, $c=8{\cdot}556$ Å, $\beta=118{\cdot}405°$. The crystal structure was solved by a three-dimensional Patterson synthesis and refined by three-dimensional least-squares to a final R value of 0·042. The two thiophene rings make an angle of 96° to each other. The glycollic bridge connecting the thiophene rings with the quinuclidine is almost planar. The quinuclidine skeleton is twisted 5° around its threefold axis. An intermolecular hydrogen bond is present between the hydroxyl hydrogen atom of the glycollic bridge and the nitrogen atom in the quinuclidine.

Introduction

The crystal structure of the anticholinergic drug, quinuclidinyl di-α,α′-thienylglycollate,

$$(C_4H_3S)_2C(OH)CO_2C_7H_{12}N,$$

has been solved as part of our programme on the correlation between molecular configuration and pharmacological action of psychotomimetic compounds. The crystal structure of the closely related quinuclidinyl benzilate has been determined in the hydrobromide salt (Meyerhöffer & Carlström, 1969). As one of the important factors in psychotomimetic drugs is probably the availability of a free electron pair on a nitrogen atom (Gabel & Abood, 1965), it was regarded as important to solve the structure of a psychoactive base. All attempts to determine the structure of the base of the benzilate proved unsuccessful. For this reason the equally active thiophene compound was chosen as it could be analyzed directly by the 'heavy-atom' method. Another advantage was that the hydrogen positions could be determined, which was not possible in the case of the hydrobromide salt because of the strong interference of the heavy bromine atoms.

Experimental

The synthesis of quinuclidinyl di-α,α′-thienylglycollate has been described by Nyberg, Östman & Wallerberg (1970). Large, colourless, optically perfect crystals were prepared through recrystallization in acetone during slow cooling. The unit-cell dimensions were determined from Weissenberg photographs and from diffractometer measurements. The density of single crystals was established by flotation in mixed solvents.

Crystal data

Quinuclidinyl di-α,α′-thienylglycollate, $C_{17}H_{19}NO_3S_2$ F.W. 349·47

$a=9{\cdot}762\pm0{\cdot}005$ Å
$b=11{\cdot}348\pm0{\cdot}005$ Å
$c=8{\cdot}556\pm0{\cdot}005$ Å
$\beta=118{\cdot}405°\pm0{\cdot}010°$
$V=833{\cdot}72$ Å^3
D_m $1{\cdot}393\pm0{\cdot}005$ g.cm^{-3}
D_x $(Z=2)$ $1{\cdot}392\pm0{\cdot}002$ g.cm^{-3}

The only systematic absences were $0k0$ when k is odd. Since the molecule is asymmetric and the unit cell contains two molecules the space group can only be $P2_1$.

Intensity data were collected with a Philips automatic single-crystal diffractometer (PAILRED) using monochromatic Mo $K\alpha$ radiation. The crystal, having the dimensions $0{\cdot}42\times0{\cdot}62\times0{\cdot}41$ mm, was oriented about the b axis and 15 layers corresponding to the entire Cu sphere were recorded. There were 2171 independent reflexions of which 146 were too weak to be observed. The unobserved reflexions were given half the intensity of the threshold value. The intensities were corrected for corresponding background, α_1–α_2 separation, Lorentz and polarization factors, but not for extinction or absorption. The structure amplitudes were placed approximately on an absolute scale by Wilson statistics. The above calculations were performed with the program system of Ringertz (1969). The X-ray 63 program system (Stewart & High, 1965) was used during the following procedures except for the perspective drawing, which was computed with the *ORTEP* program (Johnson, 1965). All calculations were carried out on an IBM 7090 computer.

Determination of the structure

A three-dimensional Patterson function was calculated from the corrected set of diffractometer data. In the Harker section $y=\frac{1}{2}$, two heavy peaks were located. All four combinations of these two peaks were tried as S–S rotation peaks, but calculations of structure amplitudes showed essentially no differences in the reliability indices R ($R=\sum|F_o-F_c|/\sum|F_c|$) between the different alternatives. Instead a combination of one of the heavy peaks with another peak having roughly half the intensity of the first chosen caused a marked drop in the R value, indicating that the true S positions had been found. The electron density map, based upon the sulphur signs only, showed, together with the sulphur maxima, additional peaks in the vicinity of these maxima and one of the five-membered rings could be identified. Iterated Fourier refinement gave the other five-membered ring and finally the entire molecule. The R value at this stage was 0·19 with an overall temperature factor $B=3{\cdot}5$ Å^2. It was now possible to interpret correctly the Patterson function; one of the two heavy peaks in the Harker section $y=\frac{1}{2}$ was found to be composed of three coincident vectors, namely O–O, S–O and S–C.

Refinement procedure

The initial refinement was carried out by a block-diagonal three-dimensional least-squares program because of the large number of parameters involved. However, for the final refinement a full-matrix program was used. In this case the refinement had to be carried out in two steps. Initially only the strongest 1650 of the 2171 reflexions were used and the structure amplitudes were

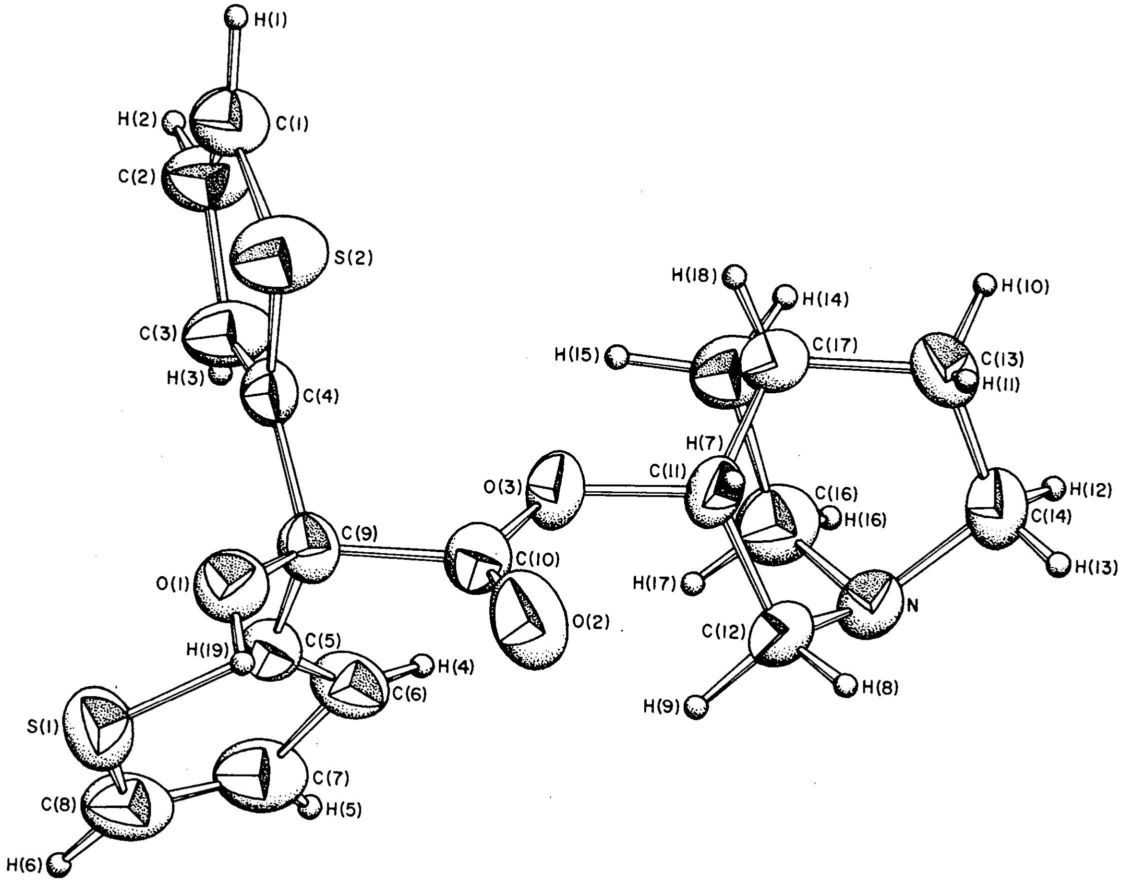

Fig. 1. A perspective drawing of the quinuclidinyl di-α,α′-thienylglycollate molecule, showing the ellipsoids of thermal motion with a probability of 50%.

Table 1. *Observed and calculated structure factors* (× 10).

Asterisks indicate unobserved reflexions

H	K	L	FO	FC	AC	BC
13	0	-5	20	12	-12	0
12	6	-5	29	28	-28	2
12	5	-8	15	27	-24	-13
12	5	-7	23	26	-20	17
12	5	-6	49	44	-34	29
12	5	-5	34	39	-36	15
12	5	-4	34	34	-15	-31
12	5	-3	43	44	9	-43
12	5	-2*	7	14	-4	-13
12	4	-8	33	30	8	-29
12	4	-7	76	73	73	8
12	4	-6	33	34	19	-28
12	4	-5	67	65	29	-58
12	4	-4	47	42	4	-42
12	4	-3	19	17	11	13
12	4	-2	21	14	-14	1
12	3	-8	59	61	55	-27
12	3	-7	40	37	14	-34
12	3	-6	37	36	-8	-35
12	3	-5	15	14	-3	14
12	3	-4*	7	10	8	6
12	3	-3	17	9	6	-6
12	3	-2	29	30	3	-30
12	2	-8	66	61	7	60
12	2	-7	49	46	12	44
12	2	-6	37	40	-13	38
12	2	-5	71	66	59	30
12	2	-4	17	14	-14	-1
12	2	-3	14	12	-9	9
12	2	-2	57	55	11	54
12	1	-8	31	25	13	21
12	1	-7	28	23	12	-20
12	1	-6	27	26	17	19
12	1	-5	20	29	28	9
12	1	-4*	7	9	-3	9
12	1	-3	88	86	72	48
12	1	-2	14	7	7	1
12	0	-8	17	18	-18	0
12	0	-7	67	58	-58	0
12	0	-6	17	11	-11	0
12	0	-5	34	36	-36	0
12	0	-4	14	2	2	0
12	0	-3	17	16	-16	0
12	0	-2	44	50	-50	0
11	8	-6	49	51	4	51
11	8	-5	31	26	-7	25
11	8	-4	19	14	-12	7
11	8	-3	15	15	-9	12
11	7	-7	27	26	26	-4
11	7	-6	36	35	-6	34
11	7	-5	26	11	-11	-1
11	7	-4	24	12	-12	-4
11	7	-3	17	13	-4	12
11	7	-2	40	32	25	20
11	6	-8	36	39	-25	-30
11	6	-7*	7	7	-4	-6
11	6	-6	81	79	-79	7
11	6	-5	52	53	-34	-40
11	6	-4	40	38	-26	-28
11	6	-3	34	33	31	-11
11	6	-2	18	15	-14	5
11	5	-9	38	35	-2	-35
11	5	-8	28	27	26	-8
11	5	-7	41	38	-16	35
11	5	-6	17	19	-7	-17
11	5	-5*	7	14	-11	-9
11	5	-4*	7	20	-16	-13
11	5	-3	42	39	-39	-3
11	5	-2	43	46	-17	-42
11	5	-1	20	20	-7	19
11	4	-9	79	80	53	-59
11	4	-8	61	57	54	18
11	4	-7	59	62	56	-28
11	4	-6	20	18	-11	-15
11	4	-5	42	40	38	-29
11	4	-4*	7	26	-15	21
11	4	-3	67	68	62	-27
11	4	-2	47	47	47	0
11	4	-1*	7	14	-14	-1
11	3	-9	24	12	-1	-12
11	3	-8*	7	7	-6	2
11	3	-7	42	43	-42	9
11	3	-6	39	39	33	21
11	3	-5	7	21	21	-3
11	3	-4	35	33	24	-23
11	3	-3	32	37	35	-12
11	3	-2	46	47	-46	-10
11	3	-1	34	25	-17	-18
11	2	-9	28	28	8	27
11	2	-8	50	51	7	50
11	2	-7	86	84	42	73
11	2	-6	37	39	36	16
11	2	-5	42	44	14	41
11	2	-4	34	35	-18	29
11	2	-3	32	32	1	32
11	2	-2	27	26	18	19
11	2	-1	17	16	0	-16
11	1	-9	26	22	9	-20
11	1	-8	35	28	12	26
11	1	-7*	7	12	6	10
11	1	-6	23	18	-2	18
11	1	-5	24	21	-4	21
11	1	-4	45	48	36	33
11	1	-3	23	28	22	18
11	1	-2	30	36	3	-36
11	1	-1	49	52	38	35
11	0	-9	13	11	-11	0
11	0	-8	68	70	-70	0
11	0	-7	35	39	-39	0
11	0	-6	78	76	-76	0
11	0	-5	40	50	-50	0
11	0	-4	80	77	-77	0
11	0	-3	67	66	-66	0
11	0	-2*	7	7	7	0
11	0	-1	44	48	48	0
10	10	-4	7	12	9	-9
10	10	-3	30	24	23	-7
10	9	-7	31	21	-21	-2
10	9	-6	23	26	15	21
10	9	-5	17	13	-12	-3
10	9	-4	21	21	16	-14
10	9	-3	22	29	22	18
10	9	-2	29	31	1	-31
10	8	-8	37	32	-20	25
10	8	-7	27	31	20	24
10	8	-6	40	43	-23	37
10	8	-5	18	21	-20	-8
10	8	-4	39	40	-8	40
10	8	-3	19	11	2	10
10	8	-2	59	57	-18	54
10	8	-1	46	44	-26	35
10	7	-8*	7	11	9	7
10	7	-7	30	26	-25	7
10	7	-6	40	47	-47	-3
10	7	-5	10	9	5	7
10	7	-4	38	38	36	-11
10	7	-3	29	28	1	28
10	7	-2	16	11	-4	-10
10	7	-1	30	26	23	12
10	6	-9	14	17	-17	5
10	6	-8	30	30	-27	11
10	6	-7	45	40	-37	-15
10	6	-6	61	62	-60	-14
10	6	-5	70	78	-7	-77
10	6	-4	54	48	-30	-37
10	6	-3	70	77	-37	-67
10	6	-2*	7	11	6	-9
10	6	-1	32	31	-31	3
10	5	-10	30	31	28	-14
10	5	-9	15	30	28	9
10	5	-8	17	10	7	8
10	5	-7*	7	16	16	4
10	5	-6	40	52	-3	-52
10	5	-5*	7	6	-4	5
10	5	-4	28	30	5	-30
10	5	-3	34	30	22	21
10	5	-2	59	62	-38	49
10	5	-1	46	46	-43	17
10	4	-10	34	27	21	-16
10	4	-9	23	27	122	-24
10	4	-8	48	51	47	-20
10	4	-7	59	65	58	-31
10	4	-6	59	57	55	-56
10	4	-5	87	86	86	-3
10	4	-4	22	30	22	20
10	4	-3	24	23	20	11
10	4	-2	20	18	10	-15
10	4	-1	33	33	33	-5
10	3	-10	34	31	-8	30
10	3	-8	40	34	7	34
10	3	-7	32	26	-26	-1
10	3	-6	32	26	17	19
10	3	-5	42	43	-43	-3
10	3	-4	35	34	4	-34
10	3	-3	40	41	40	10
10	3	-2	35	35	28	-22
10	3	-1	26	15	9	-12
10	2	-10	49	51	15	49
10	2	-9	63	63	35	52
10	2	-8	67	66	-8	66
10	2	-7	58	57	19	54
10	2	-6	25	27	-26	6
10	2	-5	67	61	52	32
10	2	-4	49	50	36	34
10	2	-3	55	83	69	47
10	2	-2	23	27	27	-4
10	2	-1	25	28	-26	10
10	1	-10	21	12	-3	12
10	1	-9	44	38	-14	-35
10	1	-8	25	21	-18	11
10	1	-7	46	42	-30	-30
10	1	-6	30	27	-25	-11
10	1	-5*	7	16	-4	15
10	1	-4	32	30	-14	-26
10	1	-3	47	51	38	34
10	1	-2	35	34	18	-29
10	1	-1	90	88	24	85
10	0	-10	30	31	-31	0
10	0	-9	27	21	-21	0
10	0	-8	85	89	-89	0
10	0	-7	36	38	-38	0
10	0	-6	96	98	-98	0
10	0	-5	69	68	-68	0
10	0	-4	64	61	-61	0
10	0	-3	31	30	-30	0
10	0	-2	64	66	-66	0
10	0	-1	38	40	-40	0
9	11	-5	17	12	9	7
9	11	-4	18	12	-6	-10
9	11	-3	23	26	4	26
9	11	-2	13	18	-18	4
9	10	-7	33	29	29	-5
9	10	-6	35	33	26	19
9	10	-5	20	19	19	-2
9	10	-4	28	31	18	25
9	10	-3	35	30	30	5
9	10	-2	46	40	40	2
9	10	-1	30	30	12	-28
9	9	-8	15	18	3	18
9	9	-7*	7	14	-6	13
9	9	-6*	7	12	11	2
9	9	-5	23	22	-16	15
9	9	-4	23	21	18	-10
9	9	-3	37	36	-16	32
9	9	-2	49	47	-34	-33
9	9	-1*	7	9	1	9
9	8	-9	44	47	31	36
9	8	-8	21	23	-23	2
9	8	-7*	7	15	-6	14
9	8	-6	55	57	-43	38
9	8	-5	25	26	8	24
9	8	-4	50	45	-12	44
9	8	-3	54	51	-31	41
9	8	-2	35	31	10	29
9	8	-1	14	16	-11	11
9	7	-9	29	28	-10	-26
9	7	-8	37	32	-32	-1
9	7	-7	45	41	-31	-26
9	7	-6	16	24	2	-24
9	7	-5	58	57	32	-48
9	7	-4	45	48	-21	-43
9	7	-3	30	33	15	29
9	7	-2	26	21	17	-13
9	7	-1	43	44	-28	34
9	6	-9	14	17	-15	-8
9	6	-8	56	59	-26	-54
9	6	-7	56	56	-3	-56
9	6	-6	83	82	-76	-29
9	6	-5	50	56	5	-56
9	6	-4	66	66	-31	59
9	6	-3	43	46	-25	-38
9	6	-2	59	56	-54	-16
9	6	-1	68	66	-55	-36
9	5	-10	41	42	36	-22
9	5	-9	43	34	18	-30
9	5	-8	42	42	42	-2
9	5	-7	14	21	15	15
9	5	-6	54	53	52	10
9	5	-5	111	114	42	106
9	5	-4	71	68	20	-66
9	5	-3	35	32	-30	13
9	5	-2	31	31	-23	21
9	5	-1	28	25	5	24
9	4	-10	22	17	13	-11
9	4	-9	21	23	22	-6
9	4	-8	25	19	7	-18
9	4	-7	58	55	48	-27
9	4	-6	26	24	-16	-17
9	4	-5	113	110	105	-31
9	4	-4	46	48	30	-37
9	4	-3	81	86	85	15
9	4	-2	52	52	51	-13
9	4	-1	56	51	-4	-51
9	3	-10	74	66	-14	67
9	3	-9	47	43	-41	11
9	3	-8	61	52	-11	51
9	3	-7	46	53	-16	51
9	3	-6	51	45	44	-10
9	3	-5	41	45	42	-16
9	3	-4	37	39	14	-37
9	3	-3	20	18	-15	9
9	3	-2	115	119	-97	-69
9	3	-1	52	52	33	40
9	2	-10	35	24	16	18
9	2	-9	50	48	43	21
9	2	-8	81	84	-3	84
9	2	-7	50	51	51	3
9	2	-6	62	61	-25	56
9	2	-5	48	48	6	46
9	2	-4	54	57	-32	45
9	2	-1	73	70	25	65
9	2	-2	103	103	51	90
9	2	-1	62	63	38	50
9	1	-11	24	24	3	-24
9	1	-10	33	35	-29	-20
9	1	-9	53	52	-33	-40
9	1	-8	24	22	-22	5
9	1	-7	92	93	-91	-18
9	1	-6	63	62	-62	5
9	1	-5	22	22	2	-21
9	1	-4	73	66	-66	-8
9	1	-3	75	75	-0	75
9	1	-2	45	46	9	-46
9	1	-1	49	53	53	1
9	0	-11	60	53	-53	0
9	0	-10*	7	20	-20	0
9	0	-9	22	20	-20	0
9	0	-8	76	75	-75	0
9	0	-7	14	19	-19	0
9	0	-6	18	10	-10	0
9	0	-5	81	80	-80	0
9	0	-4	132	132	-132	0
9	0	-3	44	46	-46	0
9	0	-2	17	18	-18	0
9	0	-1	121	121	-121	0
8	12	-5*	7	15	-13	-7
8	12	-4	24	23	-22	6
8	12	-3	16	19	-12	-15
8	12	-2	36	27	16	-22
8	11	-7	38	36	8	35
8	11	-6	36	30	23	20
8	11	-5	39	42	-12	40
8	11	-4	32	27	2	-27
8	11	-3	40	41	36	17
8	11	-2	45	44	-30	-31
8	11	-1	36	35	28	21
8	10	-8	39	37	-4	37
8	10	-7	69	65	65	-5
8	10	-6	20	20	-3	20
8	10	-5	41	38	36	-13
8	10	-4	22	25	19	15
8	10	-3*	7	15	6	-14
8	10	-2	20	26	22	-15
8	10	-1	25	28	28	-4
8	9	-8	13	21	19	9
8	9	-7	24	27	-27	0
8	9	-6	27	26	-14	22
8	9	-5	34	28	-21	18
8	9	-4	45	45	-44	-9
8	9	-3	52	45	-16	42
8	9	-2	33	31	-25	-18
8	9	-1	22	24	6	24
8	8	-9*	7	12	11	-5
8	8	-8	50	51	-51	9
8	8	-7	38	39	-7	38
8	8	-6	27	26	-5	26
8	8	-5	28	29	-11	-27
8	8	-4	76	78	3	77
8	8	-3	51	53	-29	44
8	8	-2	13	21	12	16
8	8	-1	54	57	-47	34
8	7	-9	40	37	-22	-30
8	7	-8	20	10	-10	-1
8	7	-7	52	52	14	-50
8	7	-6	76	77	-6	-77
8	7	-5	24	15	-14	-4
8	7	-4	50	55	-43	-34
8	7	-3	39	43	40	-14
8	7	-2	20	25	6	-24
8	7	-1	34	33	-18	27
8	6	-10	[illegible]	25	0	-25
8	6	-9	23	26	18	21
8	6	-8	34	33	-17	-29
8	6	-7*	7	13	-10	-6
8	6	-6	73	79	-75	24
8	6	-5	77	75	42	-63
8	6	-4	50	57	-46	-34
8	6	-3	37	40	-28	-29
8	6	-2	76	76	-77	0
8	6	-1	75	75	-72	-21
8	5	-11	40	36	17	-34
8	5	-10	57	53	35	43
8	5	-9	14	14	14	1
8	5	-8	54	49	48	10
8	5	-7	51	51	51	1
8	5	-6	67	67	55	-38
8	5	-5	21	30	30	-4
8	5	-4	32	34	-1	34
8	5	-3	164	168	30	165
8	5	-2	51	48	12	46
8	5	-1	86	87	54	-69
8	4	-11	22	22	-13	18
8	4	-10*	7	19	18	7
8	4	-9	27	33	22	-25
8	4	-8	12	17	9	14
8	4	-7	67	69	20	-62
8	4	-6	59	59	-35	-48
8	4	-5	139	108	108	0
8	4	-4	50	56	51	23
8	4	-3	199	202	121	-162
8	4	-2	113	115	6	-115
8	4	-1	50	50	32	-36
8	3	-11	34	32	29	12
8	3	-10	67	65	23	61
8	3	-9	62	65	-38	53
8	3	-8	98	95	17	94
8	3	-7	71	72	-68	24
8	3	-6	37	42	-14	-39
8	3	-5	50	51	-34	38
8	3	-4	54	49	47	-13
8	3	-3	54	55	-52	18
8	3	-2	67	70	-40	57
8	3	-1	94	98	67	72
8	2	-11	15	24	24	5
8	2	-10	15	8	6	-4
8	2	-9	51	50	10	49
8	2	-8	69	70	-65	25
8	2	-7	36	40	-40	5
8	2	-6	63	63	-18	60
8	2	-5	171	167	42	162
8	2	-4	96	100	63	77
8	2	-3	55	56	37	42
8	2	-2	91	88	72	51
8	2	-1	108	113	-90	68
8	1	-11	33	28	-10	-26
8	1	-10	55	53	-52	-10
8	1	-9	56	47	-31	-35
8	1	-8	76	76	-75	-12
8	1	-7	74	70	-21	-66
8	1	-6	38	36	-4	-34
8	1	-5	101	102	-102	3
8	1	-4	121	121	-35	-115
8	1	-3	80	79	-13	78
8	1	-2	101	103	-96	-35
8	1	-1	110	117	-37	111
8	0	-11	15	25	25	0
8	0	-10	31	32	-32	0
8	0	-9	16	12	-12	0
8	0	-6	59	58	-58	0
8	0	-7	116	113	113	0
8	0	-6	154	156	-156	0
8	0	-5	60	55	55	0
8	0	-4*	7	6	-6	0
8	0	-3	87	86	-66	0
8	0	-2	141	145	-145	0
8	0	-1	82	80	-80	0
7	13	-3	26	23	23	2
7	12	-6	54	53	-48	21
7	12	-5	35	33	-25	-21
7	12	-3	23	26	13	-23
7	12	-2	25	20	-7	-19
7	12	-1*	7	2	-1	-2
7	11	-7	34	28	4	28
7	11	-6	42	39	34	18
7	11	-5	45	41	18	37
7	11	-4*	7	17	10	-13
7	11	-3	29	26	13	22
7	11	-2*	7	13	2	-13
7	11	-1	73	72	71	14
7	10	-8	15	17	16	7
7	10	-7	32	37	34	-12
7	10	-6	42	39	-24	31
7	10	-5	16	21	19	-9
7	10	-4	25	28	18	22
7	10	-3	26	25	23	-10
7	10	-2	39	40	23	-33
7	10	-1	40	38	-31	-21
7	9	-9	26	22	-22	-3
7	9	-8	32	32	-23	22
7	9	-7	60	61	-61	5
7	9	-6*	7	6	-3	-5
7	9	-5	40	38	-17	34
7	9	-4	43	43	-43	5
7	9	-3	39	38	-35	15
7	9	-2	55	62	-61	-7
7	9	-1	78	77	-19	75
7	8	-9	21	17	-2	16
7	8	-8	64	64	-64	-8
7	8	-7	61	66	54	-25
7	8	-6	53	52	-50	15
7	8	-5*	7	7	3	6
7	8	-4	56	58	33	48
7	8	-3	44	41	7	41
7	8	-2	86	89	6	89
7	8	-1	24	24	-6	23
7	7	-10	22	24	15	19
7	7	-9	52	49	-27	-41
7	7	-8	57	58	19	-54
7	7	-7	77	71	-38	-60
7	7	-6	44	42	1	-42
7	7	-5	69	71	68	-20
7	7	-4	79	78	9	-78
7	7	-3	70	72	-42	58
7	7	-2	130	133	-94	-94
7	7	-1	33	30	11	-27
7	6	-10*	7	5	4	3
7	6	-9	15	25	9	-24
7	6	-8	43	41	-39	-10
7	6	-7*	7	10	0	10
7	6	-6	64	66	34	56
7	6	-5	78	80	35	-72
7	6	-4	180	185	-139	123
7	6	-3	157	165	-130	-102
7	6	-2	56	58	28	-51
7	6	-1	96	95	-40	-86
7	5	-11	21	22	21	-7
7	5	-10	23	25	22	11
7	5	-9	26	21	9	20
7	5	-8	61	57	52	-21
7	5	-7	49	50	42	26
7	5	-6	83	85	53	-67
7	5	-5	131	131	92	93
7	5	-4	65	59	50	-32
7	5	-3	45	50	50	6
7	5	-2	111	112	67	-90
7	5	-1	73	81	71	-37
7	4	-11	28	24	11	22
7	4	-10	28	24	-68	18
7	4	-9	41	38	-1	39
7	4	-8	60	60	-47	-39
7	4	-7	81	83	20	-80
7	4	-6	111	115	105	-46
7	4	-5	183	180	178	29
7	4	-4	223	220	-99	-196
7	4	-3	64	62	-60	17
7	4	-2	58	58	58	-1
7	4	-1	14	22	9	20
7	3	-11*	7	11	-1	-11
7	3	-11	117	115	-44	106
7	3	-9	22	22	-22	-1
7	3	-8	63	58	-25	53
7	3	-7	29	34	13	31
7	3	-6	106	100	39	93
7	3	-5	163	169	-103	134
7	3	-4	142	142	-136	42
7	3	-3	246	253	24	252
7	3	-2	41	41	34	-24
7	3	-1*	7	7	-7	3
7	2	-11	16	16	-11	-11
7	2	-10	31	30	1	30
7	2	-9	47	46	-3	-46
7	2	-8	65	68	-67	-9
7	2	-7	110	115	115	7
7	2	-6	160	155	-92	124
7	2	-5	41	48	20	43
7	2	-4	139	144	17	143
7	2	-3	118	115	56	101
7	2	-2	70	73	-53	51
7	2	-1	96	96	34	90
7	1	-11	30	30	-28	10
7	1	-10	62	64	-57	-29
7	1	-9	95	92	-47	-79
7	1	-8	28	34	16	-30
7	1	-7	77	73	-22	-70
7	1	-6	64	68	-27	-62
7	1	-5	43	40	-39	6
7	1	-4	53	58	-58	-9
7	1	-3	90	88	-86	18
7	1	-2	194	192	-64	-173
7	1	-1	32	35	35	-4
7	0	-11	26	13	-13	0
7	0	-10	28	25	-25	0
7	0	-9	25	27	27	0
7	0	-8*	7	15	15	0
7	0	-7	46	47	47	0
7	0	-6	17	14	-14	0
7	0	-5	47	43	43	0
7	0	-4	83	82	-82	0
7	0	-3	108	103	-103	0
7	0	-2	94	97	-97	0
7	0	-1	265	275	-275	0
6	13	-5	19	4	0	4
6	13	-4	30	30	-4	-29
6	13	-3	25	29	28	7
6	13	-2	30	30	-24	-19
6	13	-1	39	37	31	-21
6	12	-6	48	47	-2	47
6	12	-5	21	[illegible]	[illegible]	[illegible]
6	12	-4	20	23	6	[illegible]
6	12	-3	51	48	-32	-36
6	12	-2	35	30	25	-16
6	12	-1	16	6	-6	1
6	11	-8	51	49	35	34
6	11	-7	49	42	19	36
6	11	-6	41	41	39	-10
6	11	-5	18	18	-6	17
6	11	-4	16	5	-9	2
6	11	-3	63	60	37	47
6	11	-2	28	25	23	-7
6	11	-1	25	27	27	1
6	10	-8	40	43	-42	9
6	10	-7	54	55	37	-42
6	10	-6	31	34	-24	23
6	10	-5	14	18	9	-15
6	10	-4*	7	6	-6	3
6	10	-3	17	20	2	-19
6	10	-2	30	29	-27	-11
6	10	-1	30	34	-22	26
6	9	-9	66	69	-69	4
6	9	-8*	7	7	-1	-7
6	9	-7	33	31	-30	11
6	9	-6	41	37	-36	6
6	9	-5	57	59	-53	26
6	9	-4	57	56	-44	35
6	9	-3	127	125	5	125
6	9	-2	35	33	-32	5
6	9	-1	56	61	59	17
6	8	-9*	7	15	13	-8
6	8	-8	20	5	-7	-5
6	8	-7	37	36	36	6
6	8	-6*	7	6	-4	4
6	8	-5	42	43	39	18
6	8	-4	90	96	25	95
6	8	-3	66	87	-73	-47
6	8	-2	121	122	90	-82
6	8	-1	92	96	-54	80
6	7	-10	13	22	21	4
6	7	-9	56	50	0	-50
6	7	-8	23	9	-3	-8
6	7	-7	41	50	48	-14
6	7	-6	65	66	-18	-64
6	7	-5	64	66	-66	-5
6	7	-4	174	174	-123	-123
6	7	-3	79	63	12	-62
6	7	-2	140	149	5	-149
6	7	-1	36	39	1	39
6	6	-10*	7	10	-3	-10
6	6	-9	24	23	17	16
6	6	-8	44	36	-28	26
6	6	-7	56	60	60	-1
6	6	-6	62	62	-59	-18
6	6	-5	62	65	0	65
6	6	-4	136	135	-129	39
6	6	-3	179	173	61	-162
6	6	-2	61	63	-11	-62
6	6	-1	55	58	-52	-27
6	5	-11	22	18	-1	-18
6	5	-10	72	70	39	59
6	5	-9	56	55	13	-54
6	5	-8	104	106	97	-52
6	5	-7	81	80	64	-48
6	5	-6	108	105	82	66
6	5	-5	103	108	4	108
6	5	-4	154	152	13	-152
6	5	-3	129	131	128	27
6	5	-2	117	118	84	-84
6	5	-1	115	115	106	46
6	4	-11	18	23	11	20
6	4	-10	17	17	-17	-4
6	4	-9	24	17	-6	-16
6	4	-8	40	38	-37	12
6	4	-7	95	93	82	44
6	4	-6	154	150	-88	131
6	4	-5	176	172	25	-170
6	4	-4	69	69	-44	-53
6	4	-3	126	127	125	-18
6	4	-2	32	26	6	-28
6	4	-1	35	26	-19	-18
6	3	-11	22	23	-14	18
6	3	-10	52	46	-29	36
6	3	-9	56	50	-49	8
6	3	-8	103	99	41	90
6	3	-7	148	149	-100	111
6	3	-6	84	85	-75	41
6	3	-5	255	258	-29	257
6	3	-4	59	59	13	57
6	3	-3	125	129	7	129
6	3	-2	92	92	-90	22
6	3	-1	232	236	102	213
6	2	-11	24	22	-18	-13
6	2	-10	61	61	-35	-50
6	2	-9	63	63	8	-63
6	2	-8	35	31	31	2
6	2	-7	25	31	30	9
6	2	-6	92	92	-16	98
6	2	-5	66	81	81	5
6	2	-4	125	119	59	-104
6	2	-3	108	187	-182	42
6	2	-2	232	229	180	141
6	2	-1	90	96	-10	96
6	1	-11	52	52	-26	-45
6	1	-10	55	57	-54	-17
6	1	-9	70	70	70	-7
6	1	-8	27	27	-27	2
6	1	-7	87	81	-10	-80
6	1	-6	103	107	2	-107
6	1	-5	147	145	-107	-96
6	1	-4	229	229	-176	-147
6	1	-3	127	123	122	15
6	1	-2	172	176	-74	-160
6	1	-1	109	104	-103	-19
6	0	-11	10	18	18	0
6	0	-10	16	11	11	0
6	0	-9	59	64	64	0
6	0	-8	113	115	-115	0
6	0	-7	82	78	78	0
6	0	-6	159	164	-164	0
6	0	-5*	7	0	0	0
6	0	-4	111	107	-107	0
6	0	-3	76	73	73	0
6	0	-2	187	176	-176	0
6	0	-1**	7	10	-10	0
5	13	-5*	7	10	2	10
5	13	-4	56	53	6	-53
5	13	-3	37	34	34	-4
5	13	-2	30	29	1	-28
5	13	-1	22	21	18	-11
5	12	-7*	7	15	6	-14
5	12	-6	39	38	-7	37
5	12	-5	7	23	14	-19
5	12	-4	16	12	9	8
5	12	-3*	7	2	-2	1
5	12	-2*	7	9	4	8
5	12	-1	35	34	-17	-29
5	11	-8	30	29	26	-12
5	11	-7	18	16	5	15
5	11	-6*	7	9	9	-3
5	11	-5	59	56	11	55
5	11	-4	53	51	45	-25
5	11	-3	54	51	24	44
5	11	-2	46	50	-37	-33
5	11	-1	65	64	43	47
5	10	-8	48	54	-54	6
5	10	-7	36	36	0	-36
5	10	-6	58	59	-57	28
5	10	-5	75	73	47	-56
5	10	-4*	7	15	11	10
5	10	-3	68	67	-67	5
5	10	-2	44	43	42	9
5	10	-1	100	98	33	93
5	9	-9	33	40	-37	15
5	9	-8	24	11	-7	8
5	9	-7	51	50	-50	6
5	9	-6	29	30	-24	19
5	9	-5	57	61	13	60

Table 1 (*cont.*)

H	K	L	FO	FC	AC	BC
5	9	-5	57	61	13	60
5	9	-4	70	70	-68	16
5	9	-3	70	75	67	34
5	9	-2	33	31	-4	31
5	9	-1	102	105	13	104
5	8	-9	35	36	34	12
5	8	-8*	7	8	-8	-3
5	8	-7	60	59	57	-15
5	8	-6	16	19	-19	2
5	8	-5	60	64	39	-51
5	8	-4	63	61	-31	-52
5	8	-3	72	72	-25	-68
5	8	-2	103	103	52	90
5	8	-1	138	136	-80	110
5	7	-10	35	31	31	-2
5	7	-9	50	52	-41	-32
5	7	-8	32	29	22	-19
5	7	-7	31	31	-17	-26
5	7	-6	55	52	-41	-32
5	7	-5	64	67	-67	-2
5	7	-4	210	211	-80	-195
5	7	-3	54	54	36	-41
5	7	-2	200	201	-41	-197
5	7	-1	99	99	1	-99
5	6	-10	16	19	-8	17
5	6	-9	21	28	24	-14
5	6	-8	19	22	-6	21
5	6	-7	69	69	66	19
5	6	-6	115	116	-50	105
5	6	-5	131	131	-62	-116
5	6	-4*	7	7	4	-6
5	6	-3	65	67	54	-39
5	6	-2	138	135	33	131
5	6	-1	35	38	-35	-15
5	5	-11	20	19	0	19
5	5	-10	27	27	18	22
5	5	-9	54	54	24	-48
5	5	-8	64	63	63	8
5	5	-7	84	87	23	84
5	5	-6	145	149	52	-140
5	5	-5	171	174	172	-26
5	5	-4	113	120	116	30
5	5	-3	191	196	157	118
5	5	-2	60	68	67	-12
5	5	-1	70	79	55	57
5	4	-11	39	39	-33	22
5	4	-10	50	49	-50	3
5	4	-9	50	52	-13	50
5	4	-8	25	28	-23	17
5	4	-7	47	47	44	18
5	4	-6	51	50	-20	-46
5	4	-5	47	51	-30	41
5	4	-4	87	87	-86	15
5	4	-3	135	139	51	129
5	4	-2	52	46	45	-4
5	4	-1	124	121	-48	111
5	3	-11	20	30	-20	-22
5	3	-10	33	31	-10	30
5	3	-9	74	77	60	-48
5	3	-8	81	79	-18	77
5	3	-7	130	133	129	35
5	3	-6	143	145	-49	136
5	3	-5	252	252	-11	252
5	3	-4	76	69	68	13
5	3	-3	227	230	52	295
5	3	-2	100	87	81	-31
5	3	-1	59	63	-22	59
5	2	-11*	7	16	-8	-14
5	2	-10	33	32	14	-29
5	2	-9	45	49	39	-29
5	2	-8	51	52	-49	-17
5	2	-7	143	148	109	-99
5	2	-6	27	23	-12	-20
5	2	-5	153	157	107	-115
5	2	-4	173	172	-170	-28
5	2	-3	54	51	-48	18
5	2	-2	33	33	31	22
5	2	-1	209	195	-120	-154
5	1	-11	22	20	-13	-15
5	1	-10	29	23	3	23
5	1	-9	57	55	-48	-28
5	1	-8	94	90	-40	-80
5	1	-7	83	87	-70	-52
5	1	-6	113	116	-113	-28
5	1	-5	173	166	160	45
5	1	-4	214	211	80	-195
5	1	-3	240	242	-241	-24
5	1	-2	463	454	-295	-345
5	1	-1	104	105	-105	-4
5	0	-11	15	24	24	0
5	0	-10	36	37	-37	0
5	0	-9	40	37	37	0
5	0	-8	89	90	-90	0
5	0	-7	60	60	60	0
5	0	-6	58	55	-55	0
5	0	-5	227	218	218	0
5	0	-4	53	59	-59	0
5	0	-3	410	385	-385	0
5	0	-2	214	208	208	0
5	0	-1	82	79	79	0
4	14	-3	16	6	-5	3
4	14	-2	13	10	-9	-4
4	14	-1*	7	17	-17	-4
4	13	-6	20	15	4	-14
4	13	-5	27	22	21	6
4	13	-4	49	48	-22	-42
4	13	-3	50	48	39	28
4	13	-2	64	67	-31	-59
4	13	-1	66	67	48	-47
4	12	-7*	7	6	1	-6
4	12	-6	33	33	17	28
4	12	-5	36	36	-1	-36
4	12	-4	42	43	-11	42
4	12	-3	43	42	-29	30
4	12	-2	31	28	16	-23
4	12	-1	57	53	-7	53
4	11	-8	23	13	5	-12
4	11	-7*	7	11	1	-11
4	11	-6	37	38	29	-25
4	11	-5	32	35	7	35
4	11	-4	35	34	23	25
4	11	-3	45	46	33	35
4	11	-2	55	51	37	35
4	11	-1	52	52	19	49
4	10	-8	64	63	-62	-3
4	10	-7	46	41	23	-34
4	10	-6	55	55	-51	19
4	10	-5	26	26	25	-6
4	10	-4	36	35	-11	36
4	10	-3	22	24	-21	12
4	10	-2	66	82	79	21
4	10	-1	45	50	-39	32
4	9	-9	27	21	-15	15
4	9	-8	25	16	16	2
4	9	-7	42	41	-25	33
4	9	-6	27	30	-8	29
4	9	-5	65	67	-40	54
4	9	-4	50	47	-34	-32
4	9	-3	86	86	55	66
4	9	-2	131	130	-130	-3
4	9	-1	86	83	-63	54
4	8	-9	41	38	38	-1
4	8	-8	14	13	13	-3
4	8	-7	59	60	58	-13
4	8	-6	62	64	-64	3
4	8	-5	100	102	-27	-99
4	8	-4	65	67	1	-67
4	8	-3	120	122	-40	-115
4	8	-2	38	37	30	-22
4	8	-1	107	106	103	-25
4	7	-10	22	17	13	-11
4	7	-9	44	48	-33	-35
4	7	-8	34	36	36	-8
4	7	-7	65	66	-62	21
4	7	-6	130	136	-112	-78
4	7	-5	32	30	21	-21
4	7	-4	116	145	-11	-144
4	7	-3	15	17	-6	16
4	7	-2	181	186	-76	-170
4	7	-1	22	23	-21	-9
4	6	-10*	7	12	-3	-12
4	6	-9	56	52	51	-6
4	6	-8	30	34	-12	32
4	6	-7	71	73	73	-3
4	6	-6	38	39	-3	39
4	6	-5	99	100	79	62
4	6	-4	120	119	16	118
4	6	-3	60	57	32	46
4	6	-2	91	91	64	64
4	6	-1	62	59	-59	9
4	5	-11	17	22	-12	-18
4	5	-10	32	33	32	8
4	5	-9	44	46	14	-44
4	5	-8	85	82	55	61
4	5	-7	55	56	34	45
4	5	-6	117	119	102	-62
4	5	-5	117	122	85	87
4	5	-4	193	194	87	-173
4	5	-3	176	176	174	24
4	5	-2	51	49	46	-16
4	5	-1	210	213	16	212
4	4	-11*	7	5	2	-4
4	4	-10	43	40	-40	2
4	4	-9	32	29	9	27
4	4	-8	126	122	-111	51
4	4	-7	52	50	1	50
4	4	-6	125	131	-121	51
4	4	-5	50	43	-3	-43
4	4	-4	96	102	-28	98
4	4	-3	123	113	97	57
4	4	-2	74	72	53	-48
4	4	-1	54	58	-41	50
4	3	-11	31	35	-8	-33
4	3	-10	25	22	22	6
4	3	-9*	7	13	-7	-10
4	3	-8	51	51	-34	37
4	3	-7	112	117	55	103
4	3	-6	77	76	63	42
4	3	-5	151	154	-83	129
4	3	-4	241	240	-171	-169
4	3	-3	279	279	76	268
4	3	-2	224	223	-186	-123
4	3	-1	361	363	92	35
4	2	-11	16	8	-8	-1
4	2	-10*	7	16	-11	-11
4	2	-9	73	75	40	-63
4	2	-8	69	65	60	26
4	2	-7	100	106	57	-90
4	2	-6	190	194	-169	-96
4	2	-5	227	224	-141	-174
4	2	-4	143	137	-137	8
4	2	-3	135	127	-126	15
4	2	-2	374	372	185	-322
4	2	-1	98	81	-24	77
4	1	-11	19	19	2	-19
4	1	-10	22	25	-22	11
4	1	-9	36	34	-30	-17
4	1	-8	95	98	-97	16
4	1	-7	80	85	-80	-29
4	1	-6	118	123	-122	-14
4	1	-5	154	150	-146	34
4	1	-4	299	303	-191	-236
4	1	-3	336	329	-198	-262
4	1	-2	163	162	99	-128
4	1	-1	198	197	-110	164
4	0	-11	14	8	-8	0
4	0	-10*	7	7	7	0
4	0	-9	62	66	66	0
4	0	-8	17	22	-22	0
4	0	-7	161	165	165	0
4	0	-6	160	162	-162	0
4	0	-5	77	81	81	0
4	0	-4	89	84	84	0
4	0	-3	429	420	420	0
4	0	-2	372	375	374	0
4	0	-1	137	129	129	0
3	14	-4	16	18	12	13
3	14	-3	15	8	-1	-8
3	14	-2	30	32	23	-22
3	14	-1	14	16	16	-3
3	13	-6	28	25	6	-25
3	13	-5	37	37	20	31
3	13	-4	31	31	1	-31
3	13	-3	28	27	27	-1
3	13	-2	57	58	-26	-52
3	13	-1	27	23	3	23
3	12	-7	34	32	18	-27
3	12	-6	47	42	8	41
3	12	-5*	7	11	3	-10
3	12	-4	37	34	0	34
3	12	-3	37	33	-21	26
3	12	-2	31	34	16	30
3	12	-1	55	53	-12	52
3	11	-8	15	17	1	-17
3	11	-7	26	18	-12	14
3	11	-6	21	23	19	-13
3	11	-5	70	70	55	43
3	11	-4	59	62	35	-51
3	11	-3	79	82	58	58
3	11	-2	20	18	10	15
3	11	-1	30	34	21	26
3	10	-8	69	62	-56	26
3	10	-7	28	29	18	-23
3	10	-6	58	56	-41	36
3	10	-5	72	71	-14	-70
3	10	-4	23	25	-19	17
3	10	-3	73	71	-45	55
3	10	-2	42	43	42	9
3	10	-1	80	81	-75	30
3	9	-9	19	22	4	22
3	9	-8	28	27	19	20
3	9	-7	38	43	-16	40
3	9	-6	81	80	-60	-43
3	9	-5	21	25	-6	-25
3	9	-4	52	50	-50	-3
3	9	-3	27	35	-27	23
3	9	-2	159	161	-161	-2
3	9	-1	48	46	-3	46
3	8	-9	29	31	31	6
3	8	-8	27	29	-17	-23
3	8	-7	56	54	-3	-54
3	8	-6	69	74	-47	-57
3	8	-5	51	57	31	-47
3	8	-4	69	71	-13	-70
3	8	-3	60	56	-41	-38
3	8	-2	68	68	68	-4
3	8	-1	100	107	-58	-90
3	7	-10*	7	10	-5	-8
3	7	-9	34	31	-29	-10
3	7	-8*	7	10	10	-1
3	7	-7	63	64	-60	23
3	7	-6	64	63	-32	-54
3	7	-5	79	81	63	50
3	7	-4	102	103	-38	-96
3	7	-3	120	121	73	96
3	7	-2	170	176	27	-174
3	7	-1	66	62	-21	58
3	6	-10	39	42	5	42
3	6	-9	61	64	52	37
3	6	-8	56	57	0	57
3	6	-7	112	114	102	-51
3	6	-6	31	30	-25	16
3	6	-5	131	143	143	0
3	6	-4	162	166	149	72
3	6	-3	186	183	134	126
3	6	-2	217	211	-13	211
3	6	-1	196	194	-112	159
3	5	-10	38	39	18	34
3	5	-9	30	29	-22	-19
3	5	-8	51	51	23	46
3	5	-7	90	91	-1	-91
3	5	-6	60	71	47	-52
3	5	-5	156	163	152	57
3	5	-4	184	185	111	-148
3	5	-3	187	192	153	117
3	5	-2	72	70	-32	63
3	5	-1	205	200	193	-52
3	4	-10	31	26	-25	-7
3	4	-9	18	15	11	11
3	4	-8	57	60	-59	6
3	4	-7	75	78	-63	46
3	4	-6	202	206	-196	62
3	4	-5	29	30	-18	-24
3	4	-4	100	105	-16	104
3	4	-3	47	40	39	8
3	4	-2	42	36	30	20
3	4	-1	136	137	-135	-18
3	3	-10	56	52	46	23
3	3	-9	29	29	28	-7
3	3	-8	43	43	-34	27
3	3	-7	101	103	-80	65
3	3	-6	34	34	1	-34
3	3	-5	100	100	-44	87
3	3	-4	102	98	18	-96
3	3	-3	334	334	-55	330
3	3	-2	209	206	-203	-36
3	3	-1	353	356	-110	338
3	2	-11	16	13	-5	12
3	2	-10	32	31	-22	-22
3	2	-9	21	21	12	-17
3	2	-8	110	111	-109	-22
3	2	-7	93	91	-28	-86
3	2	-6	54	59	-58	-10
3	2	-5	215	219	44	-214
3	2	-4	138	140	-68	-122
3	2	-3	117	119	-94	-63
3	2	-2	123	127	42	-120
3	2	-1	452	455	-455	-1
3	1	-11*	7	17	-4	-17
3	1	-10	35	32	-23	22
3	1	-9	42	44	-39	-21
3	1	-8	42	45	-44	-10
3	1	-7	92	93	-76	55
3	1	-6	116	119	30	-115
3	1	-5	94	91	11	-90
3	1	-4	146	156	-21	-155
3	1	-3	409	408	-163	374
3	1	-2	71	71	67	-25
3	1	-1	309	316	-312	-47
3	0	-11*	7	11	11	0
3	0	-10	51	46	46	0
3	0	-9	111	114	114	0
3	0	-8	41	43	-43	0
3	0	-7	224	225	225	0
3	0	-6	79	75	75	0
3	0	-5	304	305	305	0
3	0	-4	118	120	120	0
3	0	-3	157	171	171	0
3	0	-2	565	574	574	0
3	0	-1	457	462	-462	0
2	14	-4	26	27	20	19
2	14	-3	15	22	9	-20
2	14	-2	31	32	17	-26
2	14	-1*	7	13	8	11
2	13	-6*	7	11	-5	-10
2	13	-5	32	28	18	21
2	13	-4	53	54	-32	-43
2	13	-3	28	23	12	25
2	13	-2	24	27	-24	-13
2	13	-1	45	49	48	10
2	12	-7	42	41	11	-39
2	12	-6	42	40	19	35
2	12	-5*	7	8	6	-6
2	12	-4	73	71	5	70
2	12	-3	55	56	27	50
2	12	-2	43	48	38	-30
2	12	-1	36	36	-24	28
2	11	-7	17	15	-2	15
2	11	-6	42	37	37	0
2	11	-5	41	37	19	32
2	11	-4	38	40	40	-5
2	11	-3	45	51	20	47
2	11	-2	40	43	-13	-41
2	11	-1	20	20	13	16
2	10	-8	52	48	-45	18
2	10	-7	35	31	19	-24
2	10	-6	77	77	-75	18
2	10	-5	13	4	-3	-3
2	10	-4	81	82	-70	42
2	10	-3	99	99	-98	-9
2	10	-2	53	60	4	-60
2	10	-1	152	160	-159	-20
2	9	-8	22	21	5	-20
2	9	-7	25	24	-5	23
2	9	-6	24	21	-18	-11
2	9	-5	40	45	40	21
2	9	-4	146	144	-121	-77
2	9	-3	62	65	-50	42
2	9	-2	150	159	-153	-46
2	9	-1	59	68	17	66
2	8	-9	50	50	13	-49
2	8	-8	47	52	-50	-13
2	8	-7	43	43	31	-29
2	8	-6*	7	13	13	0
2	8	-5	115	114	63	-95
2	8	-4	47	46	0	46
2	8	-3	65	67	65	-17
2	8	-2	111	117	103	-57
2	8	-1	106	112	-51	-100
2	7	-9	47	47	-47	3
2	7	-8	26	31	31	-7
2	7	-7	14	9	-8	-4
2	7	-6	119	120	95	-74
2	7	-5	122	118	53	106
2	7	-4	50	53	-53	6
2	7	-3	108	109	61	90
2	7	-2	215	212	-210	-27
2	7	-1	66	62	-53	-31
2	6	-10	19	19	-6	18
2	6	-9	40	38	38	-5
2	6	-8	30	31	31	3
2	6	-7	83	86	84	-16
2	6	-6	81	81	34	74
2	6	-5	115	115	115	-11
2	6	-4	173	174	151	86
2	6	-3	126	119	-92	75
2	6	-2	108	112	111	9
2	6	-1	74	69	31	-62
2	5	-10	17	16	3	-15
2	5	-9	45	42	-39	16
2	5	-8	50	53	-27	46
2	5	-7*	7	8	-2	-8
2	5	-6	117	115	40	-108
2	5	-5	60	48	36	31
2	5	-4	149	149	-15	-148
2	5	-3	199	192	78	176
2	5	-2	105	103	32	-97
2	5	-1	61	57	32	-47
2	4	-10	33	36	-35	11
2	4	-9	22	18	4	18
2	4	-8	95	94	-81	48
2	4	-7*	7	14	-2	13
2	4	-6	151	155	-154	-19
2	4	-5	212	211	-108	181
2	4	-4	216	212	-25	211
2	4	-3	289	283	-281	32
2	4	-2	274	265	-191	-184
2	4	-1	196	201	-161	120
2	3	-10	31	31	4	31
2	3	-9*	7	10	7	-8
2	3	-8	54	50	-3	50
2	3	-7	92	95	95	-3
2	3	-6	113	112	-71	-87
2	3	-5	180	178	-35	174
2	3	-4	155	163	-144	-77
2	3	-3	311	310	-253	179
2	3	-2	164	167	-153	-68
2	3	-1	394	398	163	363
2	2	-10	29	27	-14	-23
2	2	-9	18	13	12	-4
2	2	-8	89	92	-76	-51
2	2	-7	167	168	2	-168
2	2	-6	121	125	118	-41
2	2	-5	20	28	21	-19
2	2	-4	87	86	-82	26
2	2	-3	217	213	175	-122
2	2	-2	400	407	40	-405
2	2	-1	256	275	-190	-199
2	1	-10	29	26	11	23
2	1	-9	24	31	-18	-25
2	1	-8	21	20	10	-18
2	1	-7	32	29	2	29
2	1	-6	119	115	115	-3
2	1	-5	71	74	-18	72
2	1	-4	278	278	194	-199
2	1	-3	90	95	37	87
2	1	-2	305	313	-56	-307
2	1	-1	577	598	-571	176
2	0	-10	32	30	30	0
2	0	-9	76	79	79	0
2	0	-8	20	11	11	0
2	0	-7	203	210	210	0
2	0	-6	47	43	-43	0
2	0	-5	289	292	292	0
2	0	-4	158	165	165	0
2	0	-3*	7	19	19	0
2	0	-2	369	379	379	0
2	0	-1	622	624	-624	0
1	15	-1	30	38	24	30
1	14	-4	34	33	28	-19
1	14	-3	21	23	3	-23
1	14	-2	43	43	42	7
1	14	-1	20	25	25	5
1	13	-5	18	19	-1	19
1	13	-4	58	55	-44	-34
1	13	-3	33	35	26	24
1	13	-2	37	42	-13	-40
1	13	-1	21	28	26	9
1	12	-6	57	52	0	52
1	12	-5	21	18	-16	9
1	12	-4	50	49	37	33
1	12	-3	18	18	13	-12
1	12	-2	22	25	-9	-23
1	12	-1	101	115	-8	115
1	11	-7	21	22	9	20
1	11	-6	31	25	-21	-14
1	11	-5*	7	11	-5	10
1	11	-4	52	50	-43	-26
1	11	-3	31	29	-20	21
1	11	-2*	7	4	-4	-1
1	11	-1	74	88	87	-8
1	10	-8	16	10	-2	10
1	10	-7	33	32	-12	-30
1	10	-6	95	92	-87	31
1	10	-5	72	70	-62	-34
1	10	-4	81	81	-80	6
1	10	-3	62	64	-62	-13
1	10	-2	53	50	5	-50
1	10	-1	159	169	-168	24
1	9	-8*	7	8	7	-3
1	9	-7	20	19	-11	15
1	9	-6	40	40	7	-40
1	9	-5	51	46	32	33
1	9	-4	29	26	-26	7
1	9	-3	34	29	28	9
1	9	-2	19	18	-9	16
1	9	-1	43	47	44	17
1	8	-9	22	11	-2	-11
1	8	-8	28	28	-17	-22
1	8	-7	80	75	67	-32
1	8	-6	21	21	-17	12
1	8	-5	53	53	50	15
1	8	-4	117	117	110	-38
1	8	-3	64	68	18	-65
1	8	-2	120	125	75	-100
1	8	-1	177	184	-16	-183
1	7	-9	39	35	24	25
1	7	-8	46	46	36	-29
1	7	-7	50	50	-42	27
1	7	-6	63	62	22	-58
1	7	-5	122	124	89	86
1	7	-4	160	161	-50	-153
1	7	-3	147	151	-15	151
1	7	-2	117	115	-52	-103
1	7	-1	33	41	27	30
1	6	-9	43	44	43	-10
1	6	-8	54	53	-53	-3
1	6	-7	49	52	52	-4
1	6	-6	37	40	39	5
1	6	-5	173	171	167	-33
1	6	-4	33	36	-13	33
1	6	-3	123	116	-27	113
1	6	-2	193	188	143	-122
1	6	-1	157	162	13	162
1	5	-10	28	28	0	28
1	5	-9	56	53	-43	-31
1	5	-8	22	30	1	30
1	5	-7	75	77	-56	-53
1	5	-6	75	78	-71	31
1	5	-5	119	115	-43	106
1	5	-4	104	102	-93	-43
1	5	-3	85	86	60	61
1	5	-2	265	267	79	-255
1	5	-1	375	371	344	138
1	4	-10	15	19	-12	-15
1	4	-9	40	42	26	33
1	4	-8	130	130	-113	63
1	4	-7	56	54	-54	0
1	4	-6	181	182	-70	169
1	4	-5	80	82	35	74
1	4	-4	169	169	-165	-35
1	4	-3	326	317	-258	-185
1	4	-2	367	366	-56	362
1	4	-1	358	377	-369	78
1	3	-10	25	27	-3	27
1	3	-9	42	45	-45	3
1	3	-8	58	58	5	-58
1	3	-7	89	90	86	26
1	3	-6	148	148	31	-144
1	3	-5	105	95	-32	90
1	3	-4	215	214	-69	-203
1	3	-3	507	495	84	487
1	3	-2	93	101	-35	-95
1	3	-1	174	168	167	-22
1	2	-10	22	26	-23	-13
1	2	-9	56	56	-6	-56
1	2	-8	87	90	-80	-42
1	2	-7	125	125	93	-83
1	2	-6	43	48	-7	-47
1	2	-5	180	177	52	-169
1	2	-4	242	227	209	-91
1	2	-3	225	228	-120	-194
1	2	-2	308	308	-170	-257
1	2	-1	827	870	-539	683
1	1	-10	22	19	-5	19
1	1	-9	16	21	20	-7
1	1	-8	60	62	52	33
1	1	-7	116	111	110	15
1	1	-6	107	109	-4	-109
1	1	-5	30	28	25	-13
1	1	-4	39	39	30	25
1	1	-3	297	301	-67	293
1	1	-2	163	172	-110	132
1	1	-1	292	296	166	-246
1	0	-10	21	16	16	0
1	0	-9	54	53	53	0
1	0	-8	16	19	19	0
1	0	-7	25	27	27	0
1	0	-6	94	96	-96	0
1	0	-5	215	220	220	0
1	0	-4*	7	3	3	0
1	0	-3	336	338	338	0
1	0	-2	605	623	623	0
1	0	-1	228	211	-211	0
0	0	1	30	28	28	0
0	0	2	214	212	212	0
0	0	3	164	151	-151	0
0	0	4	102	103	103	0
0	0	5	23	24	-24	0
0	0	6	22	9	9	0
0	0	7	130	132	132	0
0	0	8	84	83	-83	0
0	0	9	28	28	28	0
0	0	10*	7	9	-9	0
0	1	1	520	516	514	-40
0	1	2	499	497	-93	488
0	1	3	58	60	13	-59
0	1	4	133	132	-127	36
0	1	5	229	229	83	-213
0	1	6	156	157	-126	94
0	1	7	91	92	58	-71
0	1	8	44	45	-32	-32
0	1	9	33	28	-17	-22
0	1	10	19	26	-25	-8
0	2	0	267	267	-117	-238
0	2	1	189	194	-162	-106
0	2	2	291	276	-264	81
0	2	3	438	428	-288	-317
0	2	4	102	104	-57	-88
0	2	5	207	207	175	-109
0	2	6	48	50	-49	-13
0	2	7	64	70	68	-16
0	2	8	48	55	-37	-40
0	2	9	30	27	-5	-26
0	2	10	37	43	-9	-42
0	3	1	162	168	141	-92
0	3	2	302	301	34	299
0	3	3	116	113	-112	-10
0	3	4	158	153	-153	7
0	3	5	165	165	-87	-140
0	3	6	116	115	75	87
0	3	7	89	88	-50	73
0	3	8	59	59	-43	41
0	3	9	87	85	-25	81
0	4	0	120	118	60	102
0	4	1	225	239	-238	-24
0	4	2	112	106	22	-104
0	4	3	315	310	-218	220
0	4	4	164	167	-148	77
0	4	5	107	105	-102	-23
0	4	6	100	102	-37	95
0	4	7	75	76	71	26
0	4	8	21	20	-18	-9
0	4	9	25	22	21	-5
0	5	1	123	123	47	114
0	5	2	191	190	91	167
0	5	3	169	164	-5	-164
0	5	4	198	192	105	160
0	5	5	118	117	43	-109
0	5	6	109	108	42	-99
0	5	7	37	32	32	4
0	5	8	39	38	15	35
0	5	9	33	39	31	-24
0	6	0	212	210	204	48
0	6	1	197	197	44	192
0	6	2	305	290	281	74
0	6	3	70	74	61	-41
0	6	4	52	52	22	46
0	6	5	90	88	-5	88
0	6	6	18	20	7	19
0	6	7	38	39	39	0
0	6	8	49	46	-10	45
0	6	9	24	18	18	-6
0	7	1	98	95	-85	-42
0	7	2	102	102	30	97
0	7	3	33	35	-35	-5
0	7	4	151	145	145	7
0	7	5	105	105	45	-95
0	7	6	83	83	-76	30
0	7	7	24	24	-21	-11
0	7	8	17	22	-15	16
0	7	9	25	27	22	16
0	8	0	51	52	11	-51
0	8	1	87	94	-36	-87
0	8	2	213	217	44	-213
0	8	3	36	36	-33	-14
0	8	4	29	29	-2	28
0	8	5	92	97	90	-34
0	8	6	15	18	-6	-17
0	8	7	71	74	48	-57
0	8	8*	7	12	-8	-9
0	9	1	117	124	-124	-2
0	9	2	22	20	-20	-1
0	9	3	119	118	-97	-68
0	9	4	59	62	56	27
0	9	5	105	99	-93	-34
0	9	6	54	52	-9	52
0	9	7	66	66	-65	-15
0	9	8*	7	9	-3	8
0	10	0	190	192	191	23
0	10	1	163	176	-145	99
0	10	2	71	70	-43	-56
0	10	3	86	84	-83	-9
0	10	4*	7	10	-9	4
0	10	5	42	38	-21	-32

Table 1 (*cont.*)

H	K	L	FO	FC	AC	BC
0	10	6	29	28	-17	22
0	10	7	25	21	6	-20
0	11	1	38	45	45	-2
0	11	2	47	49	8	48
0	11	3	47	46	-10	-45
0	11	4	53	50	45	23
0	11	5	31	32	30	-12
0	11	6	46	44	2	44
0	11	7	33	35	25	-24
0	12	0	38	36	-8	-35
0	12	1	56	59	-13	57
0	12	2	24	22	17	14
0	12	3	25	25	-22	11
0	12	4	42	39	17	35
0	12	5	31	32	32	-2
0	12	6	53	47	-7	46
0	13	1	17	17	0	-17
0	13	2	36	36	34	12
0	13	3	39	39	-19	-34
0	13	4	31	27	3	26
0	13	5•	7	13	-6	-12
0	14	0	17	15	6	-14
0	14	1•	7	7	4	-5
0	14	2	45	47	45	-16
0	14	3•	7	15	13	-7
0	15	1•	7	12	-10	-6
1	0	0	203	213	213	0
1	0	1	495	506	506	0
1	0	2	474	471	471	0
1	0	3	77	83	83	0
1	0	4•	7	5	-5	0
1	0	5	156	160	160	0
1	0	6	29	31	-31	0
1	0	7	22	18	18	0
1	0	8	18	12	-12	0
1	0	9	19	10	10	0
1	1	0	476	497	-284	-407
1	1	1	764	782	-771	-130
1	1	2	418	402	-245	319
1	1	3	109	109	-108	14
1	1	4	145	145	1144	21
1	1	5	135	138	-15	-137
1	1	6	124	124	121	-29
1	1	7	44	44	-28	-34
1	1	8•	7	8	6	-6
1	1	9	25	23	-22	2
1	2	0	600	639	128	-626
1	2	1	487	498	-339	-365
1	2	2	450	436	259	-343
1	2	3	85	73	-26	68
1	2	4	214	212	-143	-157
1	2	5	73	71	-25	-66
1	2	6	47	56	-52	-21
1	2	7	68	67	60	-29
1	2	8	44	46	-45	7
1	2	9	37	34	20	27
1	3	0	30	26	-7	-25
1	3	1	60	54	-2	-54
1	3	2	201	199	-196	-30
1	3	3	281	261	79	-249
1	3	4	338	330	53	326
1	3	5	160	157	-137	-78
1	3	6	109	105	9	105
1	3	7	28	27	3	27
1	3	8	64	69	-31	61
1	3	9	34	36	-32	17
1	4	0	100	102	-91	47
1	4	1	274	276	-228	156
1	4	2	272	262	144	219
1	4	3	211	198	-198	-6
1	4	4	60	58	6	58
1	4	5	35	34	-19	-28
1	4	6	27	31	-26	17
1	4	7	57	59	40	-44
1	4	8	25	23	-17	16
1	4	9	35	37	34	16
1	5	0	134	129	127	22
1	5	1	71	68	4	-68
1	5	2	189	185	40	180
1	5	3	40	39	5	-39
1	5	4	107	103	68	78
1	5	5	73	78	45	64
1	5	6	81	80	80	-3
1	5	7	92	93	41	-84
1	5	8	41	40	-11	-38
1	5	9	47	41	4	41
1	6	0	265	270	259	75
1	6	1	228	223	63	214
1	6	2	244	231	231	-13
1	6	3	69	68	18	66
1	6	4	101	97	67	-71
1	6	5	52	48	-26	40
1	6	6	82	82	-20	80
1	6	7	53	61	34	51
1	6	8	36	34	-21	27
1	7	0	67	67	-43	-51
1	7	1	175	173	-167	-46
1	7	2	111	106	55	-91
1	7	3	216	213	-135	-165
1	7	4	129	127	32	123
1	7	5	118	116	64	-97
1	7	6	35	33	27	19
1	7	7	56	58	-9	-57
1	7	8	16	18	-17	7
1	8	0	125	136	135	-21
1	8	1	175	175	-143	102
1	8	2	84	83	82	-14
1	8	3	207	201	-17	-201
1	8	4	115	116	-55	-102
1	8	5	57	60	-4	-60
1	8	6	45	44	-34	28
1	8	7	32	39	35	-16
1	8	8	22	18	-10	16
1	9	0	56	55	48	-27
1	9	1•	7	7	-4	-5
1	9	2	149	148	-76	127
1	9	3	107	104	-91	50
1	9	4	45	41	23	33
1	9	5	70	69	-33	-60
1	9	6	34	34	-33	10
1	9	7	13	16	-10	-15
1	10	0•	7	5	5	2
1	10	1	100	105	-43	96
1	10	2	19	16	9	-14
1	10	3	42	39	-37	-13
1	10	4	14	10	-9	-6
1	10	5	33	31	21	-22
1	10	6	45	41	-18	37
1	10	7•	7	9	8	-4
1	11	0	33	38	8	-37
1	11	1	51	52	-46	-26
1	11	2	53	51	0	51
1	11	3	21	20	-4	20
1	11	4	30	21	15	15
1	11	5	25	23	16	-17
1	11	6	59	56	48	28
1	12	0	55	54	53	-37
1	12	1	42	45	1	45
1	12	2•	7	10	6	8
1	12	3	35	34	-2	34
1	12	4•	7	9	3	8
1	12	5	16	15	-14	6
1	13	0•	7	12	8	9
1	13	1	14	16	4	-16
1	13	2	21	20	19	8
1	13	3	33	28	7	-27
1	13	4	47	41	41	8
1	14	0	31	36	23	-27
1	14	1•	7	12	-12	-8
1	14	2	21	21	7	-19
1	14	3•	7	19	-18	-3
1	15	0	16	27	-5	26
2	0	0	448	462	462	0
2	0	1	205	187	-187	0
2	0	2	384	382	382	0
2	0	3	104	102	-102	0
2	0	4	15	12	12	0
2	0	5	85	83	-83	0
2	0	6•	7	11	11	0
2	0	7	83	87	87	0
2	0	8	26	31	31	0
2	0	9	25	25	25	0
2	1	0	221	218	-208	66
2	1	1	477	463	-454	-92
2	1	2	432	412	-375	-169
2	1	3	80	84	49	-68
2	1	4	85	87	-21	85
2	1	5	205	206	-63	-197
2	1	6	56	54	-49	22
2	1	7	39	40	5	-40
2	1	8	29	33	-33	-1
2	1	9	13	17	12	-11
2	2	0	333	331	141	-300
2	2	1	85	81	14	-80
2	2	2	100	105	54	-90
2	2	3	232	222	-78	-208
2	2	4	63	58	-17	-55
2	2	5	68	76	29	-70
2	2	6	91	96	-96	-8
2	2	7	45	42	39	15
2	2	8	29	35	-9	34
2	2	9	28	25	-8	24
2	3	0	282	277	10	-276
2	3	1	47	50	50	1
2	3	2	370	364	122	343
2	3	3	53	53	-44	29
2	3	4	145	150	12	149
2	3	5	80	77	-76	14
2	3	6	40	45	-14	42
2	3	7	23	23	-21	-11
2	3	8	30	35	34	12
2	3	9	15	20	10	17
2	4	0	273	256	255	-28
2	4	1	326	309	-281	129
2	4	2	162	160	20	149
2	4	3	168	159	-65	145
2	4	4	114	113	15	112
2	4	5	56	61	-41	-44
2	4	6	56	55	-13	54
2	4	7	52	52	42	-31
2	4	8	48	49	-39	-29
2	5	0	267	258	239	95
2	5	1	266	260	201	-166
2	5	2	280	271	189	195
2	5	3	52	49	-9	-48
2	5	4	97	98	81	55
2	5	5	77	75	15	-73
2	5	6	62	65	-1	65
2	5	7	33	31	29	12
2	5	8	14	8	7	4
2	6	0	183	167	104	34
2	6	1	179	175	-143	101
2	6	2	68	67	66	-6
2	6	3	80	80	14	78
2	6	4	66	62	62	1
2	6	5	47	50	49	-8
2	6	6	44	42	-10	-41
2	6	7	27	24	24	3
2	6	8	65	66	-44	49
2	7	0	196	197	74	-183
2	7	1	136	133	52	-122
2	7	2	43	43	-33	28
2	7	3	188	181	-107	-147
2	7	4	63	63	-63	-5
2	7	5	58	57	-13	-56
2	7	6	39	35	31	-16
2	7	7	75	70	25	-65
2	7	8	30	31	-15	-27
2	8	0	150	149	98	-111
2	8	1	56	55	-18	-52
2	8	2	84	83	28	-78
2	8	3	76	76	-3	76
2	8	4	36	32	-21	-23
2	8	5	48	40	18	036
2	8	6	59	58	-57	-10
2	8	7•	7	11	5	-10
2	9	0	79	75	-35	66
2	9	1	140	145	106	99
2	9	2	37	38	31	-23
2	9	3	144	139	-138	-16
2	9	4	81	77	-18	75
2	9	5	18	17	-11	-14
2	9	6	31	36	20	30
2	9	7	19	19	-19	2
2	10	0	92	98	-13	-97
2	10	1	120	122	-90	83
2	10	2	82	84	77	33
2	10	3	41	43	-39	18
2	10	4•	7	8	7	4
2	10	5	41	38	-22	-31
2	10	6	15	12	12	-1
2	11	0	68	66	63	19
2	11	1	41	41	25	-33
2	11	2•	7	15	4	-15
2	11	3	20	17	-13	10
2	11	4	70	60	22	56
2	11	5	22	18	-18	0
2	11	6	48	46	15	44
2	12	0•	7	5	-4	-3
2	12	1	74	76	21	74
2	12	2	39	39	39	4
2	12	3	17	19	-4	19
2	12	4•	7	16	14	8
2	12	5	35	29	20	-21
2	13	0	23	27	6	-26
2	13	1•	7	10	6	-8
2	13	2	19	20	19	7
2	13	3	58	51	-13	-50
2	13	4	19	14	14	-3
2	14	0	34	35	30	-17
2	14	1	21	24	-20	12
2	14	2	14	11	10	3
3	0	0	85	89	89	0
3	0	1	289	276	-276	0
3	0	2	41	38	38	0
3	0	3	159	153	-153	0
3	0	4	63	60	60	0
3	0	5	60	59	59	0
3	0	6	30	28	-28	0
3	0	7	41	39	39	0
3	0	8	25	17	-17	0
3	1	0	239	243	-101	-221
3	1	1	315	314	92	-300
3	1	2	240	234	-117	-203
3	1	3	212	214	-122	-176
3	1	4	159	161	-57	150
3	1	5	101	107	-57	-90
3	1	6	17	18	-16	7
3	1	7	56	59	-10	-58
3	1	8	18	8	-7	-5
3	2	0	34	40	40	-4
3	2	1	143	149	-56	-138
3	2	2	355	354	311	-169
3	2	3	125	124	112	-55
3	2	4	37	32	-10	-31
3	2	5	17	15	11	10
3	2	6	70	70	-68	17
3	2	7	32	34	-16	30
3	2	8	33	32	-29	-15
3	3	0	193	193	-156	114
3	3	1	115	110	98	49
3	3	2	251	254	-79	242
3	3	3	80	82	-34	75
3	3	4	199	196	-2	196
3	3	5	57	58	-21	54
3	3	6	55	55	-1	55
3	3	7	27	21	8	-20
3	3	8	15	9	6	6
3	4	0	92	94	-68	65
3	4	1	171	169	-154	70
3	4	2	182	182	179	34
3	4	3	62	60	-56	23
3	4	4	105	100	9	100
3	4	5	35	40	-35	-19
3	4	6	36	32	-31	5
3	4	7	32	29	29	-3
3	4	8	10	14	-12	-7
3	5	0	73	75	31	-69
3	5	1	87	85	70	-49
3	5	2	127	121	121	9
3	5	3	145	142	83	-116
3	5	4	67	63	43	46
3	5	5	25	21	21	-4
3	5	6	45	48	41	25
3	5	7	15	17	17	1
3	5	8•	7	13	12	-4
3	6	0	79	76	12	-75
3	6	1	101	102	-98	28
3	6	3	25	26	-12	23
3	6	4	127	127	51	-116
3	6	5	45	48	-41	23
3	6	6•	7	5	-5	-1
3	6	7	35	38	23	-31
3	7	0	125	129	-25	-127
3	7	1	136	131	-124	-41
3	7	2	62	59	34	-49
3	7	3	97	93	-37	-85
3	7	4	29	32	19	-25
3	7	5	94	88	-54	-70
3	7	6	15	10	-5	9
3	7	7	32	34	4	-33
3	8	0	207	205	116	-169
3	8	1	37	34	-16	30
3	8	2	87	87	67	55
3	8	3	17	17	-5	17
3	8	4	36	32	-22	23
3	8	5	29	27	18	-21
3	8	6	29	26	-20	16
3	8	7	37	36	-6	-36
3	9	0	107	110	-108	18
3	9	1	105	102	-102	-13
3	9	2	93	90	56	71
3	9	3	22	21	-9	19
3	9	4	65	63	-9	62
3	9	5	36	34	-31	-13
3	9	6	37	38	14	35
3	10	0	123	123	74	-99
3	10	1	66	65	-65	6
3	10	2	55	59	-39	-44
3	10	3	56	54	-51	18
3	10	4•	7	12	10	7
3	10	5•	7	7	5	-5
3	10	6	25	21	-5	20
3	11	0	22	25	6	24
3	11	1	80	81	79	19
3	11	2	55	50	48	16
3	11	3•	7	12	-2	-12
3	11	4	60	54	16	52
3	11	5	31	32	-18	-27
3	12	0	41	41	34	-23
3	12	1	14	37	-21	30
3	12	2	36	33	32	9
3	12	3•	7	11	6	9
3	12	4•	7	12	12	2
3	13	0•	7	15	-10	-12
3	13	1	52	48	21	-43
3	13	2	23	15	0	15
3	13	3	26	20	-17	-11
3	14	0	18	12	12	-2
3	14	1	15	12	-11	0
4	0	0	131	125	-125	0
4	0	1	334	335	-335	0
4	0	2	23	19	19	0
4	0	3•	7	12	12	0
4	0	4	60	59	59	0
4	0	5	19	18	-18	0
4	0	6•	7	17	-17	0
4	0	7	28	25	-25	0
4	1	0	160	163	-103	-126
4	1	1	84	85	-81	-26
4	1	2	65	61	-45	-41
4	1	3	197	204	-92	-182
4	1	4	79	84	80	-26
4	1	5	88	88	-46	-75
4	1	6	22	26	-21	16
4	1	7	31	33	-31	-11
4	2	0	151	152	145	-47
4	2	1	224	224	-224	8
4	2	2•	7	16	13	-9
4	2	3	170	165	44	159
4	2	4	79	78	8	77
4	2	5	23	25	24	6
4	2	6	27	28	-27	3
4	2	7	21	25	24	-7
4	3	0	237	237	-27	235
4	3	1	92	79	54	58
4	3	2	163	156	-110	110
4	3	3	68	66	-45	48
4	3	4	143	139	19	137
4	3	5	64	66	-56	35
4	3	6	93	94	-20	92
4	3	7	31	31	-30	-7
4	4	0	196	188	179	-56
4	4	1	191	186	-186	-10
4	4	2	52	51	27	-43
4	4	3	93	100	-94	-36
4	4	4	113	120	118	18
4	4	5	33	33	10	-31
4	4	6	24	20	-11	-16
4	4	7	25	15	15	0
4	5	0	167	163	121	109
4	5	1	79	76	77	-35
4	5	2	71	74	74	6
4	5	3	133	134	28	-131
4	5	4	77	81	81	0
4	5	5	76	75	31	-69
4	5	6	36	32	18	26
4	5	7	19	19	19	0
4	6	0	103	109	104	-28
4	6	1	79	81	-78	25
4	6	2	33	34	4	-34
4	6	3	120	128	-105	74
4	6	4	45	45	43	-15
4	6	5	40	41	34	-22
4	6	6	34	29	-27	-11
4	6	7	41	42	18	-38
4	7	0	96	97	-24	-94
4	7	1	158	158	32	-155
4	7	2	105	107	97	-45
4	7	3	92	92	-54	-74
4	7	4	50	51	-42	27
4	7	5	44	43	-37	-22
4	7	6	40	44	-12	43
4	8	0	89	87	85	-17
4	8	1	96	92	-84	36
4	8	2	34	33	31	-13
4	8	3	59	58	40	41
4	8	4	15	9	-3	9
4	8	5•	7	7	7	3
4	8	6•	7	14	-3	14
4	9	0	61	67	-66	-6
4	9	1	64	67	14	65
4	9	2	41	39	-29	26
4	9	3	23	19	-16	-11
4	9	4	58	59	-46	37
4	9	5	47	37	-28	-24
4	9	6	21	19	-8	17
4	10	0	65	63	-27	-57
5	10	1	45	42	-38	-17
4	10	2	59	55	54	-12
4	10	3•	7	6	-5	3
4	10	4	30	31	12	28
4	10	5•	7	9	-7	5
4	11	0•	7	8	-2	8
4	11	1	31	32	26	10
4	11	2	57	49	41	27
4	11	3	16	15	3	-15
4	11	4	62	56	53	18
4	12	0•	7	14	-14	4
4	12	1	19	15	-14	6
4	12	2	35	36	15	-33
4	12	3	29	31	2	30
4	12	4	15	12	-12	-1
4	13	0•	7	12	-12	-1
4	13	1	20	18	9	-15
4	13	2	16	21	-5	-20
4	14	0	42	42	26	-32
5	0	0	159	160	160	0
5	0	1	173	177	-177	0
5	0	2	163	166	166	0
5	0	3	127	133	133	0
5	0	4	60	61	-61	0
5	0	5	16	16	16	0
5	0	6•	7	8	-8	0
5	0	7	17	16	-16	0
5	1	0	133	135	-127	-45
5	1	1	82	85	-66	53
5	1	2	63	61	21	-57
5	1	3	178	177	19	-176
5	1	4	88	86	-33	80
5	1	5	43	44	-33	-28
5	1	6	52	55	-37	40
5	1	7	43	45	-24	-38
5	2	0	151	152	109	106
5	2	1	167	164	-45	158
5	2	2	106	107	34	101
5	2	3	36	41	-30	-26
5	2	4	72	75	48	59
5	2	5	44	46	-1	46
5	2	6	34	33	-2	33
5	2	7	41	39	4	29
5	3	0	97	100	-99	-10
5	3	1	157	158	-37	154
5	3	2	77	76	-28	71
5	3	3	61	65	-55	35
5	3	4	36	36	-1	36
5	3	5•	7	7	3	6
5	3	6•	7	16	6	15
5	3	7•	7	14	-12	7
5	4	0	143	139	87	-108
5	4	1	40	36	-23	-27
5	4	2	67	74	74	1
5	4	3	130	132	-58	-118
5	4	4	68	69	31	-61
5	4	5	51	49	47	-12
5	4	6•	7	13	2	13
5	4	7	51	47	33	-33
5	5	0	103	100	-39	92
5	5	1	113	111	11	-111
5	5	2	148	152	95	118
5	5	3	69	71	65	-28
5	5	4	47	50	49	10
5	5	5	79	81	22	-78
5	5	6	28	21	17	13
5	5	7•	7	11	-2	11
5	6	0	85	83	83	-2
5	6	1	89	89	-88	-10
5	6	2	142	145	39	-140
5	6	3	63	65	-51	40
5	6	4	24	20	-20	1
5	6	5	13	18	-6	17
5	6	6	23	13	-13	1
5	7	0	152	159	-48	-152
5	7	1	53	54	-54	3
5	7	2•	7	15	12	-8
5	7	3	31	31	31	0
5	7	4	18	18	16	-7
5	7	5	46	44	-29	-33
5	7	6	19	16	-15	-6
5	8	0	58	57	26	-50
5	8	1	30	25	-14	-21
5	8	2	26	32	-16	-28
5	8	3	50	50	-15	48
5	8	4	47	44	8	43
5	8	5	27	25	-6	24
5	9	0	105	106	-99	37
5	9	1	74	69	-64	25
5	9	2	24	19	-17	8
5	9	3	54	50	-10	-49
5	9	4	23	22	8	21
5	9	5	32	30	-30	-2
5	10	0	57	52	49	-17
5	10	1	48	46	-46	2
5	10	2	59	60	43	-42
5	10	3•	7	14	-7	12
5	10	4	21	16	2	-15
5	11	0	55	50	-28	41
5	11	1	49	44	10	43
5	11	2	43	40	35	19
5	11	3	39	38	32	-21
5	11	4	50	45	36	27
5	12	0	53	49	37	-32
5	12	1	40	39	-35	17
5	12	2	14	15	-9	-12
5	12	3	31	30	-18	-24
5	13	0	33	32	-5	-31
5	13	1	32	26	14	-22
6	0	0	175	175	175	0
6	0	1	164	168	-168	0
6	0	2	183	189	-189	0
6	0	3	31	27	-27	0
6	0	4	23	30	30	0
6	0	5•	7	10	-10	0
6	0	6	22	13	13	0
6	1	0	119	117	-56	-103
6	1	1	25	20	8	18
6	1	2	77	77	7	76
6	1	3	149	151	-144	-47
6	1	4	25	19	18	5
6	1	5	49	47	-22	-42
6	1	6	27	31	11	29
6	2	0	156	153	134	-75
6	2	1	63	63	-33	54
6	2	2	56	58	36	46
6	2	3	69	73	-65	33
6	2	4	57	56	4	56
6	2	5	60	60	33	49
6	2	6	19	21	-21	14
6	3	0	155	155	-122	96
6	3	1	93	88	87	-16
6	3	2	40	38	-14	36
6	3	3	47	46	-26	-38
6	3	4	57	56	-53	-18
6	3	5	47	48	16	-45
6	3	6	52	51	34	38
6	4	0	132	132	55	120
6	4	1	119	119	-119	-1
6	4	2	116	123	111	-53
6	4	3	16	21	3	21
6	4	4	73	73	57	-46
6	4	5	49	49	5	-49
6	4	6	37	38	28	-27
6	5	0	95	92	92	-2
6	5	1	81	83	62	54
6	5	2	18	17	-9	-15
6	5	3•	7	11	-2	-11
6	5	4	60	62	29	55
6	5	5•	7	11	9	6
6	5	6	14	18	8	-16
6	6	0	103	108	10	-108
6	6	1	49	47	-47	-1
6	6	2	72	74	54	-50
6	6	3	39	38	-33	-18
6	6	4	23	21	-21	0
6	6	5	45	48	-45	16
6	7	0	47	48	31	-36
6	7	1	97	93	-77	-53
6	7	2	27	30	-18	-25
6	7	3	33	28	-17	-23
6	7	4	62	57	57	3
6	7	5	23	26	-5	-26
6	8	0	117	120	15	119
6	8	1	69	89	-35	82
6	8	2	25	21	21	-5
6	8	3	46	49	-43	23
6	8	4•	7	14	0	-14
6	9	0	23	29	-26	-12
6	9	1	56	55	-51	19
6	9	2	63	65	-63	15
6	9	3	22	21	18	-11
6	9	4	38	36	4	35
6	10	0	77	70	66	22
6	10	1	23	26	1	26
6	10	2	26	21	-9	-19
6	10	3	27	25	18	-17
6	11	0•	7	12	2	-12
6	11	1	20	19	17	10
6	11	2	46	40	7	40
6	11	3	42	39	-38	-9
6	12	0	40	37	22	-30
6	12	1•	7	9	7	-6
6	13	0	21	25	-24	-5
7	0	0	56	56	-56	0
7	0	1	38	37	37	0
7	0	2	49	47	47	0
7	0	3	59	63	-63	0
7	0	4	47	51	-51	0
7	0	5	49	50	-50	0
7	1	0	199	201	-151	-133
7	1	1	90	97	-96	-8
7	1	2	99	100	50	87
7	1	3	35	33	33	0
7	1	4•	7	6	-5	3
7	1	5	42	39	9	-38
7	2	0	143	144	131	60
7	2	1	46	44	-22	-38
7	2	2	60	51	51	39
7	2	3	48	50	-31	39
7	2	4	26	21	-7	19
7	2	5	18	10	-10	1
7	3	0	44	44	-44	3
7	3	1	129	131	-43	123
7	3	2	23	32	-13	-29
7	3	3•	7	11	-6	10
7	3	4	46	45	38	25
7	3	5	49	47	-38	-27
7	4	0	138	142	103	-98
7	4	1	33	41	23	34
7	4	2	91	91	88	-22
7	4	3	44	41	-37	-17
7	4	4	28	28	27	8
7	4	5	38	36	36	2
7	5	0	42	36	18	31
7	5	1	65	67	10	-66
7	5	2	70	69	50	46
7	5	3	61	58	12	-57
7	5	4	42	39	3	38
7	5	5•	7	9	-7	6
7	6	0	56	61	51	-33
7	6	1	69	67	-64	-20
7	6	2	25	29	-9	-28
7	6	3	50	53	-53	-1
7	6	4	40	35	-7	-34
7	7	0	16	15	-13	-7
7	7	1	40	45	6	44
7	7	2	18	29	-5	-28
7	7	3•	7	7	-3	7
7	7	4	41	38	-24	30
7	8	0	28	29	27	12
7	8	1	100	99	-52	85
7	8	2	20	10	-10	-2
7	8	3	29	22	-13	-17
7	9	0•	7	10	2	-10
7	9	1	25	28	28	0
7	9	2	55	55	-40	38
7	9	3	33	29	-21	-20
7	10	0•	7	11	11	-2
7	10	1	37	38	28	26
7	10	2	29	31	31	3
7	11	0	32	32	-10	-30
7	11	1•	7	10	0	-10
7	12	0	26	26	20	-17
8	0	0	53	53	-53	0
8	0	1	111	110	-110	0
8	0	2	15	10	-10	0
8	0	3	16	6	-6	0
8	0	4	19	17	-17	0
8	1	0	110	113	96	-60
8	1	1	61	62	-19	-59
8	1	2	23	23	-1	-23
8	1	3	17	10	7	-7
8	1	4	54	53	21	49
8	2	0	115	114	49	103
8	2	1	43	45	-11	44
8	2	2	82	83	67	49
8	2	3	40	41	-20	-35
8	2	4	21	20	18	-8
8	3	0	64	63	-56	-30
8	3	1	26	23	-17	15
8	3	2	66	65	-16	63

given unit weight. The atomic scattering factors were those listed in *International Tables for X-ray Crystallography* (1962).

The first two cycles of block-diagonal refinement with non-hydrogen atoms only and isotropic temperature factors yielded an R value of 0·10. When anisotropic temperature factors were introduced the R value decreased to 0·075. A Fourier difference synthesis prepared at this stage made it possible to locate all of the 19 hydrogen atoms. With the hydrogen atoms included and given isotropic temperature factors, three cycles of refinement of the non-hydrogen atoms lowered the R value to 0·036. When also the positional parameters and the individual isotropic temperature factors of the hydrogen atoms were refined for one cycle the R value decreased to 0·033. The standard deviations of the atomic parameters were now quite satisfactory. In the next step the structure amplitudes were weighted. The weighting scheme adopted was $w=(a+bF_o+cF_o^2)^{-1}$ where a, b and c were derived from a quadratic curve of best fit for $|F_o-F_c|$ as a function of F_o. The numerical values of a, b and c were $a=0{\cdot}12$, $b=0{\cdot}017$, $c=-0{\cdot}0004$ for $F_o\geq 10$ and $a=0{\cdot}282$, $b=c=0$ for $F_o<10$. A final refinement including all of the 2171 weighted structure factors resulted in $R=0{\cdot}042$, *i.e.* somewhat higher than the lowest value for the 1650 reflexions, but the standard deviations of the atomic parameters were further decreased. The average of the shift to error ratio of the parameters was 0·20 for the non-hydrogen atoms and 0·85 for the hydrogen atoms. Observed and calculated structure factors from this last cycle of refinement are listed in Table 1. The positional and thermal parameters for the final structure are given in Tables 2 and 3 respectively.

Table 2. *Final fractional atomic coordinates and their standard deviations (in parentheses)*

	x/a	y/b	z/c
S(1)	0·0594 (1)	0·3500	1·0177 (1)
S(2)	0·0114 (1)	0·4893 (1)	0·4370 (1)
O(1)	0·1598 (3)	0·5242 (2)	0·8389 (3)
O(2)	0·4397 (4)	0·4686 (4)	0·8619 (5)
O(3)	0·3416 (3)	0·3041 (3)	0·7041 (3)
N	0·6342 (3)	0·0976 (3)	0·8229 (4)
C(1)	−0·1344 (5)	0·4053 (4)	0·2803 (5)
C(2)	−0·1562 (5)	0·3076 (4)	0·3496 (5)
C(3)	−0·0536 (4)	0·2979 (4)	0·5352 (4)
C(4)	0·0466 (4)	0·3899 (3)	0·6024 (4)
C(5)	0·1678 (4)	0·3181 (3)	0·9136 (4)
C(6)	0·2262 (5)	0·2028 (4)	0·9513 (5)
C(7)	0·1756 (6)	0·1463 (5)	1·0649 (5)
C(8)	0·0876 (5)	0·2132 (5)	1·1094 (5)
C(9)	0·1767 (4)	0·4104 (3)	0·7889 (4)
C(10)	0·3366 (4)	0·3995 (4)	0·7912 (4)
C(11)	0·4863 (4)	0·2835 (4)	0·6974 (5)
C(12)	0·6058 (4)	0·2171 (4)	0·8642 (5)
C(13)	0·6004 (5)	0·1804 (5)	0·5370 (5)
C(14)	0·7027 (5)	0·1058 (5)	0·7013 (6)
C(15)	0·3748 (5)	0·0912 (4)	0·5515 (5)
C(16)	0·4851 (5)	0·0345 (4)	0·7332 (6)
C(17)	0·4461 (4)	0·2060 (4)	0·5357 (5)
H(1)	−0·176 (6)	0·430 (5)	0·157 (7)
H(2)	−0·238 (7)	0·244 (6)	0·284 (8)
H(3)	−0·058 (5)	0·239 (5)	0·582 (7)
H(4)	0·275 (4)	0·178 (4)	0·923 (5)
H(5)	0·215 (7)	0·069 (6)	1·099 (8)
H(6)	0·046 (6)	0·183 (5)	1·183 (7)
H(7)	0·522 (5)	0·360 (4)	0·684 (5)
H(8)	0·709 (4)	0·266 (4)	0·922 (5)
H(9)	0·565 (5)	0·210 (5)	0·956 (6)
H(10)	0·582 (5)	0·147 (5)	0·434 (6)
H(11)	0·651 (6)	0·256 (5)	0·549 (7)
H(12)	0·718 (6)	0·017 (5)	0·674 (7)
H(13)	0·802 (6)	0·138 (5)	0·765 (7)
H(14)	0·367 (7)	0·030 (5)	0·459 (8)
H(15)	0·268 (5)	0·117 (4)	0·541 (6)
H(16)	0·506 (7)	−0·043 (6)	0·722 (8)
H(17)	0·440 (5)	0·037 (4)	0·809 (6)
H(18)	0·379 (5)	0·254 (4)	0·438 (5)
H(19)	0·217 (6)	0·538 (5)	0·932 (6)

Description and discussion of the structure

The geometry of the molecule

The atomic nomenclature and the configuration of the molecule is illustrated in Fig. 1 which also shows the ellipsoids of thermal motion scaled to include 50 per cent probability. As can be seen, the molecule is composed of two planar α-substituted thiophene rings connected to a quinuclidine nucleus by means of an almost planar bridge, called the glycollic bridge in the following. The best planes through each of the two five-membered rings were calculated with and without the sulphur atoms included. In the former case all the atoms deviated significantly from the planes whereas only the sulphur atoms deviated significantly in the latter case. These deviations amounted to 0·010 Å for S(1) and 0·014 Å for S(2). This is slightly less than found in thenoic acid. Thus, Nardelli, Fava & Giraldi (1962) observed that the sulphur atom was displaced 0·028 Å from a plane through the carbon atoms in the ring of α-thenoic acid. Later, Hudson & Robertson (1962, 1964) confirmed this result. They found the

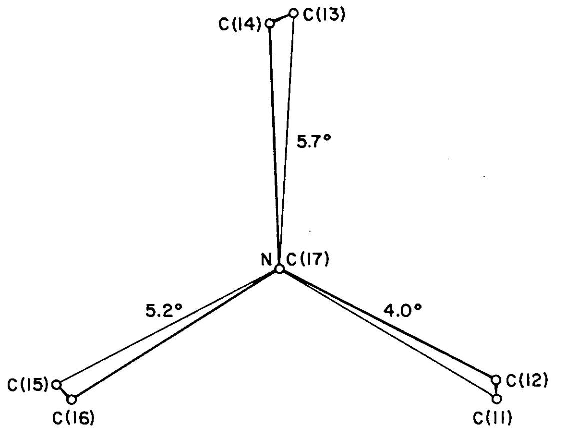

Fig. 2. The quinuclidine part of the molecule seen along its threefold axis, showing the angle of twist between the upper and lower halves.

deviation 0·02 Å of the sulphur atoms in α- and β-thenoic acids. The equations of the planes and the deviations of the atoms in the present structure are given in Table 4. The planes of the rings make an angle of 96·4° to each other.

The glycollic bridge connecting the thiophene rings to the quinuclidine part of the molecule is perfectly planar except for the hydroxyl oxygen atom, O(1), which deviates 0·34 Å from a plane defined by the atoms O(2), O(3), C(9), C(10), C(11). The equation of this plane and the atomic deviations are given in Table 4. The angles between the plane of the glycollic bridge and the thiophene rings C(1) to C(4) and C(5) to C(8) are 93° and 119° respectively.

The quinuclidine cage is almost symmetric in shape. However, when seen along its axis of symmetry, C(17)...N, it exhibits a slight distortion illustrated in Fig. 2. The mean angle of twist is 5·0 ± 0·7° which is the same as that found in our earlier investigation of the quinuclidinyl benzilate (Meyerhöffer & Carlström, 1969). The question regarding the symmetry of quinuclidine and similar cage-like structures has already been discussed in this work. Recently, a new structure determination of a bicyclo[2,2,2]octane derivative has been reported by Cameron, Ferguson & Morris (1968) who likewise observed an angle of twist (3°) about the threefold axis of the carbocycle. According to these authors the distortion is adopted solely to release strain from torsional and nonbonded intramolecular interactions.

The overall geometry of the present molecule is very similar to that of the quinuclidinyl benzilate in spite

Table 3. *Anisotropic parameters and standard deviations (in parentheses)*

β_{ij} are the coefficients in the expression $\exp\,[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)]$.

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
S(1)	0·0140 (1)	0·0099 (1)	0·0208 (2)	0·0004 (1)	0·0111 (1)	0·0007 (1)
S(2)	0·0186 (2)	0·0080 (1)	0·0183 (2)	−0·0019 (1)	0·0070 (2)	0·0030 (1)
O(1)	0·0130 (4)	0·0057 (2)	0·0159 (4)	0·0002 (2)	0·0057 (3)	−0·0023 (2)
O(2)	0·0153 (5)	0·0124 (4)	0·0289 (7)	−0·0066 (3)	0·0134 (5)	−0·0091 (5)
O(3)	0·0086 (3)	0·0064 (2)	0·0191 (5)	0·0004 (2)	0·0066 (3)	−0·0009 (3)
N	0·0098 (4)	0·0082 (3)	0·0144 (5)	0·0016 (3)	0·0051 (4)	0·0010 (3)
C(1)	0·0150 (6)	0·0100 (3)	0·0133 (6)	0·0013 (4)	0·0061 (5)	0·0007 (4)
C(2)	0·0146 (6)	0·0101 (4)	0·0135 (6)	−0·0025 (4)	0·0046 (5)	−0·0016 (4)
C(3)	0·0142 (5)	0·0068 (3)	0·0130 (5)	−0·0026 (3)	0·0037 (4)	0·0002 (3)
C(4)	0·0094 (4)	0·0055 (2)	0·0137 (5)	0·0008 (2)	0·0066 (4)	0·0002 (3)
C(5)	0·0093 (4)	0·0066 (3)	0·0112 (5)	−0·0005 (3)	0·0051 (4)	−0·0007 (3)
C(6)	0·0157 (6)	0·0067 (3)	0·0133 (6)	0·0006 (3)	0·0081 (5)	0·0014 (3)
C(7)	0·0185 (7)	0·0084 (4)	0·0156 (7)	−0·0009 (4)	0·0072 (6)	0·0019 (4)
C(8)	0·0152 (6)	0·0114 (5)	0·0132 (6)	−0·0039 (5)	0·0061 (5)	0·0010 (4)
C(9)	0·0102 (4)	0·0049 (2)	0·0143 (5)	0·0003 (3)	0·0065 (4)	−0·0007 (3)
C(10)	0·0097 (4)	0·0070 (3)	0·0144 (5)	−0·0010 (3)	0·0058 (4)	−0·0004 (3)
C(11)	0·0072 (4)	0·0075 (3)	0·0157 (6)	0·0005 (3)	0·0049 (4)	0·0005 (3)
C(12)	0·0085 (4)	0·0090 (3)	0·0132 (5)	0·0015 (3)	0·0032 (4)	−0·0001 (4)
C(13)	0·0144 (6)	0·0126 (5)	0·0167 (7)	0·0025 (4)	0·0102 (6)	0·0014 (5)
C(14)	0·0123 (5)	0·0120 (5)	0·0193 (7)	0·0036 (4)	0·0089 (5)	0·0011 (5)
C(15)	0·0119 (5)	0·0093 (4)	0·0162 (7)	−0·0010 (4)	0·0044 (5)	−0·0026 (4)
C(16)	0·0142 (6)	0·0086 (4)	0·0198 (8)	−0·0014 (4)	0·0072 (6)	0·0002 (5)
C(17)	0·0106 (5)	0·0099 (4)	0·0122 (5)	0·0019 (3)	0·0045 (4)	0·0010 (4)

Table 4. *Equations of the best planes*

The equations are of the form $m_1X+m_2Y+m_3Z=d$, X,Y,Z being the orthogonal coordinates in Å.

	Plane	m_1	m_2	m_3	d
A	C(1), C(2), C(3), C(4), S(2)	0·8587	−0·4743	−0·1941	−4·6989
B	C(1), C(2), C(3), C(4)	0·8563	−0·4787	−0·1939	−4·7087
C	C(5), C(6), C(7), C(8), S(1)	0·4995	0·3280	0·8018	5·6614
D	C(5), C(6), C(7), C(8)	0·4975	0·3308	0·8019	5·6733
E	C(9), C(10), C(11), O(2), O(3)	−0·0523	0·5289	0·8471	2·6423

Deviations (Å) from the best planes

Plane *A*		Plane *B*		Plane *C*		Plane *D*		Plane *E*	
C(1)	−0·002	C(1)	0·002	C(5)	0·004	C(5)	0·001	C(9)	−0·002
C(2)	−0·002	C(2)	−0·004	C(6)	−0·003	C(6)	−0·001	C(10)	−0·000
C(3)	0·006	C(3)	0·004	C(7)	0·000	C(7)	0·001	C(11)	−0·002
C(4)	−0·006	C(4)	−0·002	C(8)	0·002	C(8)	−0·001	O(2)	0·001
S(2)	0·004			S(1)	−0·003			O(3)	0·003
		S(2)	0·014			S(1)	−0·010		
								O(1)	0·344
								H(19)	−0·152

of the latter being a salt. The main differences are due to twists around the C(4)–C(9) and C(5)–C(9) bonds connecting the rings to the glycollic bridge, a 23° twist around the C(9)–C(10) bond and a 20° twist around the O(3)–C(11) bond. A closer comparison of the two structures seems to be of little value because of the much lower accuracy in the determination of the benzilate structure.

Bond lengths and bond angles

The bond lengths and bond angles with estimated standard deviations are listed in Tables 5 and 6 and illustrated in Fig. 3 and 4. No correction has been made for thermal motion. The thiophene rings were non-symmetric when tested with the criteria of significance proposed by Cruickshank & Robertson (1953). Thus the C(1)–C(2) bond is significantly shorter than the C(3)–C(4) bond and the same is true for corresponding bonds in the other thiophene ring. C(1)–C(2) (1·321 Å) and C(7)–C(8) (1·331 Å) are moreover slightly shorter than the standard double bond length, of 1·337 Å. Such non-symmetric thiophene rings with short C–C bonds have earlier been described by Block, Filippakis & Schmidt (1967) in α-thienylacrylic acid.

Table 5. *Interatomic distances and standard deviations (in parentheses)*

S(2)–C(4)	1·712 (4) Å	C(11)–C(12)	1·543 (5) Å
S(2)–C(1)	1·708 (4)	C(13)–C(14)	1·535 (6)
C(1)–C(2)	1·321 (7)	C(15)–C(16)	1·548 (6)
C(2)–C(3)	1·422 (5)	C(11)–C(17)	1·524 (6)
C(3)–C(4)	1·358 (5)	C(13)–C(17)	1·529 (7)
		C(15)–C(17)	1·514 (7)
S(1)–C(5)	1·714 (5)	C(12)–N	1·461 (6)
S(1)–C(8)	1·702 (5)	C(14)–N	1·483 (7)
C(8)–C(7)	1·331 (8)	C(16)–N	1·469 (6)
C(7)–C(6)	1·434 (8)		
C(6)–C(5)	1·402 (6)	C(11)–H(7)	0·96 (5)
		C(12)–H(8)	1·04 (4)
C(1)–H(1)	0·98 (6)	C(12)–H(9)	1·04 (6)
C(2)–H(2)	1·02 (6)	C(13)–H(10)	0·89 (6)
C(3)–H(3)	0·79 (6)	C(13)–H(11)	0·96 (6)
C(6)–H(4)	0·69 (5)	C(14)–H(12)	1·06 (6)
C(7)–H(5)	0·94 (6)	C(14)–H(13)	0·93 (5)
C(8)–H(6)	0·96 (7)	C(15)–H(14)	1·03 (7)
		C(15)–H(15)	1·04 (5)
C(4)—C(9)	1·511 (4)	C(16)–H(16)	0·91 (7)
C(5)—C(9)	1·527 (6)	C(16)–H(17)	0·94 (6)
C(9)—C(10)	1·556 (6)	C(17)–H(18)	0·95 (4)
C(9)—O(1)	1·395 (5)		
C(10)–O(2)	1·190 (5)	O(1)····O(2)	2·719 (5)
C(10)–O(3)	1·329 (5)	O(1)····N′	2·752 (4)
O(3)—C(11)	1·460 (5)	H(19)···O(2)	2·63 (6)
		H(19)···N′	2·02 (4)
O(1)—H(19)	0·74 (4)		

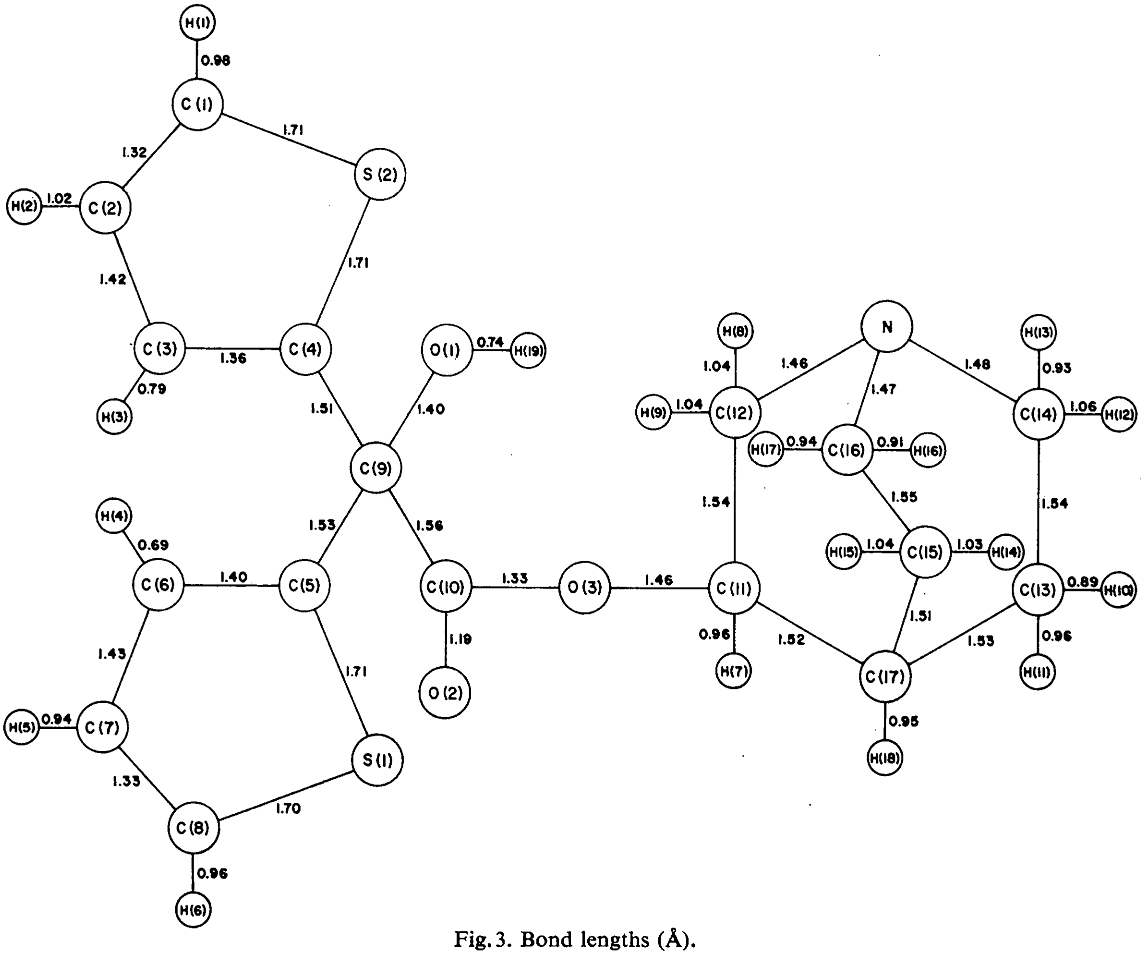

Fig. 3. Bond lengths (Å).

On comparing corresponding bond lengths in the two thiophene rings all bonds were found to be identical except for the C(3)–C(4) and C(5)–C(6) which were significantly different. Averaging the bond lengths of the thiophene rings, the mean S–C distance, 1·709 Å, is almost midway between a pure single bond, 1·815 Å and a pure double bond, 1·556 Å, as given by Bak, Christensen, Hansen-Nygaard & Rastrup-Andersen, (1961). The mean C–C bond length, 1·428 Å, opposite the sulphur atom and the mean C–C bond length, 1·353 Å, adjacent to the C–S bond deviate symmetrically with respect to the C–C bond length, 1·395 Å, of benzene. The mean bond lengths and the bond angles are all in excellent agreement with the earlier determinations of a α-substituted thiophene (Nardelli, Fava & Giraldi, 1962) as well as calculations of the thiophene structure from micro wave spectra (Bak, Christensen, Hansen-Nygaard & Rastrup-Andersen, 1961) and from electron diffraction (Momany, 1964). Large variations in bond lengths are reported for a β-substituted thiophene ring (Hudson & Robertson, 1964). On the other hand Visser, Heeres, Wolters & Vos (1968) have found normal thiophene bond lengths in α,α'- and β,β'-thienyls within the limits of the rather large experimental errors. In the rest of the molecule all bond lengths and bond angles are close to their normal values. The mean paraffinic C–C distance, 1·532 Å, the mean C–N distance, 1·471 Å and the mean C–H distance, 0·95 Å are all quite acceptable and so are the C=O and C–O bond lengths.

Hydrogen bonds and packing of the molecules

The observed planarity of the connecting glycollic bridge together with the short O(1)...O(2) distance, 2·719 Å, at first indicated the presence of an intramolecular hydrogen bond as presumed for the quinuclidinyl benzilate molecule (Meyerhöffer & Carlström, 1969). However, the short O(1)...N′$(1-x, y+\frac{1}{2}, 1-z)$

Table 6. *Interatomic angles and standard deviations* (*in parentheses*)

C(4)–S(2)–C(1)	92·6 (2)°	C(5)–S(1)–C(8)	92·4 (2)°
S(2)–C(1)–C(2)	111·6 (3)	S(1)–C(8)–C(7)	111·9 (4)
C(1)–C(2)–C(3)	112·8 (4)	C(8)–C(7)–C(6)	114·6 (5)
C(2)–C(3)–C(4)	113·3 (4)	C(7)–C(6)–C(5)	109·9 (4)
C(3)–C(4)–S(2)	109·6 (2)	C(6)–C(5)–S(1)	111·2 (3)
C(3)–C(4)–C(9)	129·8 (3)	C(6)–C(5)–C(9)	130·4 (4)
S(2)–C(4)–C(9)	120·6 (3)	S(1)–C(5)–C(9)	118·2 (3)
S(2)–C(1)–H(1)	117 (3)	S(1)–C(8)–H(6)	127 (3)
C(2)–C(1)–H(1)	131 (3)	C(7)–C(8)–H(6)	121 (3)
C(1)–C(2)–H(2)	127 (4)	C(8)–C(7)–H(5)	132 (5)
C(3)–C(2)–H(2)	121 (4)	C(6)–C(7)–H(5)	114 (5)
C(2)–C(3)–H(3)	117 (3)	C(7)–C(6)–H(4)	125 (4)
C(4)–C(3)–H(3)	130 (3)	C(5)–C(6)–H(4)	125 (4)
C(4)—C(9)—C(5)	109·5 (3)	C(11)–C(12)–N	112·1 (3)
C(4)—C(9)—C(10)	109·6 (3)	C(13)–C(14)–N	111·3 (4)
C(5)—C(9)—C(10)	109·1 (3)	C(15)–C(16)–N	111·5 (4)
C(4)—C(9)—O(1)	107·7 (3)	C(11)–C(17)–C(13)	106·0 (3)
C(5)—C(9)—O(1)	111·5 (3)	C(13)–C(17)–C(15)	109·3 (4)
C(10)–C(9)—O(1)	109·5 (3)	C(15)–C(17)–C(11)	110·3 (4)
C(9)—C(10)–O(2)	123·7 (4)	C(12)–N—C(14)	108·2 (4)
C(9)—C(10)–O(3)	111·2 (3)	C(14)–N—C(16)	109·2 (3)
O(2)—C(10)–O(3)	125·1 (4)	C(16)–N—C(12)	108·9 (3)
C(10)–O(3)—C(11)	116·6 (3)		
O(3)—C(11)–C(12)	111·2 (4)	C(9)—O(1)—H(19)	113 (4)
O(3)—C(11)–C(17)	107·0 (3)	O(3)—C(11)–H(7)	106 (3)
C(12)–C(11)–C(17)	108·3 (3)	C(12)–C(11)–H(7)	113 (2)
C(14)–C(13)–C(17)	108·7 (4)	C(17)–C(11)–H(7)	112 (3)
C(16)–C(15)–C(17)	108·5 (3)	C(11)–C(12)–H(8)	108 (2)
N——C(12)–H(8)	111 (2)	C(17)–C(15)–H(14)	113 (4)
C(11)–C(12)–H(9)	110 (3)	C(16)–C(15)–H(15)	113 (3)
N——C(12)–H(9)	107 (3)	C(17)–C(15)–H(15)	104 (3)
H(8)—C(12)–H(9)	108 (4)	H(14)–C(15)–H(15)	114 (4)
C(14)–C(13)–H(10)	114 (3)	C(15)–C(16)–H(16)	112 (4)
C(17)–C(13)–H(10)	110 (3)	N——C(16)–H(16)	108 (4)
C(14)–C(13)–H(11)	108 (3)	C(15)–C(16)–H(17)	110 (2)
C(17)–C(13)–H(11)	106 (4)	N——C(16)–H(17)	107 (2)
H(10)–C(13)–H(11)	110 (6)	H(16)–C(16)–H(17)	108 (6)
C(13)–C(14)–H(12)	115 (3)	C(11)–C(17)–H(18)	104 (3)
N——C(14)–H(12)	105 (4)	C(13)–C(17)–H(18)	112 (3)
C(13)–C(14)–H(13)	111 (4)	C(15)–C(17)–H(18)	115 (3)
N——C(14)–H(13)	107 (4)		
H(12)–C(14)–H(13)	107 (5)	O(1)–H(19)···O(2)	89 (5)
C(16)–C(15)–H(14)	105 (3)	O(1)–H(19)···N′	173 (5)

distance, 2·752 Å, seemed equally well suited to an intermolecular hydrogen bond. When the position of H(19) was established it became evident that the H(19)...O(2) distance, 2·63 Å, was much too long to permit such a bond whereas the H(19)...N′ distance, 2·02 Å was quite favourable. The existence of a hydrogen bond between O(1)H(19)...N′ is further supported by the fact that the hydrogen atom lies almost on the straight line between the oxygen atom and the nitrogen atom, the O(1)–H(19)...N′ angle being 173°. The hydrogen bond system is illustrated in Fig. 5.

The oxygen atom O(1) of the hydroxyl group is facing the sulphur atoms of the thiophene rings, the distances being as short as 2·939 Å and 3·056 Å. This verifies earlier findings that the van der Waals radius of sulphur is closer to 1·60 Å (Donohue, 1950; Nardelli, Fava & Giraldi, 1962), than to the value of 1·85 Å given by Pauling (1960) and even to the value of 1·72 Å supposed by Walker, Folting & Merritt (1969). All other distances are in accordance with ordinary requirements.

I wish to thank Professor A. Engström for his kind encouragement. To Assistant Professor D. Carlström, I am especially grateful for stimulating discussions and patient guidance throughout the whole investigation. My thanks are also due to Drs H. Ringertz and R. Bergin for helpful advice and aid in computer programming work and to Assistant Professor B. Östman for valuable criticism of the manuscript. The work was in part supported by the Swedish Medical Research Council (Project B69-11X-144-05).

References

BAK, B., CHRISTENSEN, D., HANSEN-NYGAARD, L. & RASTRUP-ANDERSEN, J. (1961). *J. Mol. Spectr.* **7**, 58.

BLOCK, S., FILIPPAKIS, S. E. & SCHMIDT, G. M. J. (1967). *J. Chem. Soc.* p. 233.

CAMERON, A. F., FERGUSON, G. & MORRIS, D. G. (1968). *Chem. Comm.* **6**, 316.

CRUICKSHANK, D. W. J. & ROBERTSON, A. P. (1953). *Acta Cryst.* **6**, 698.

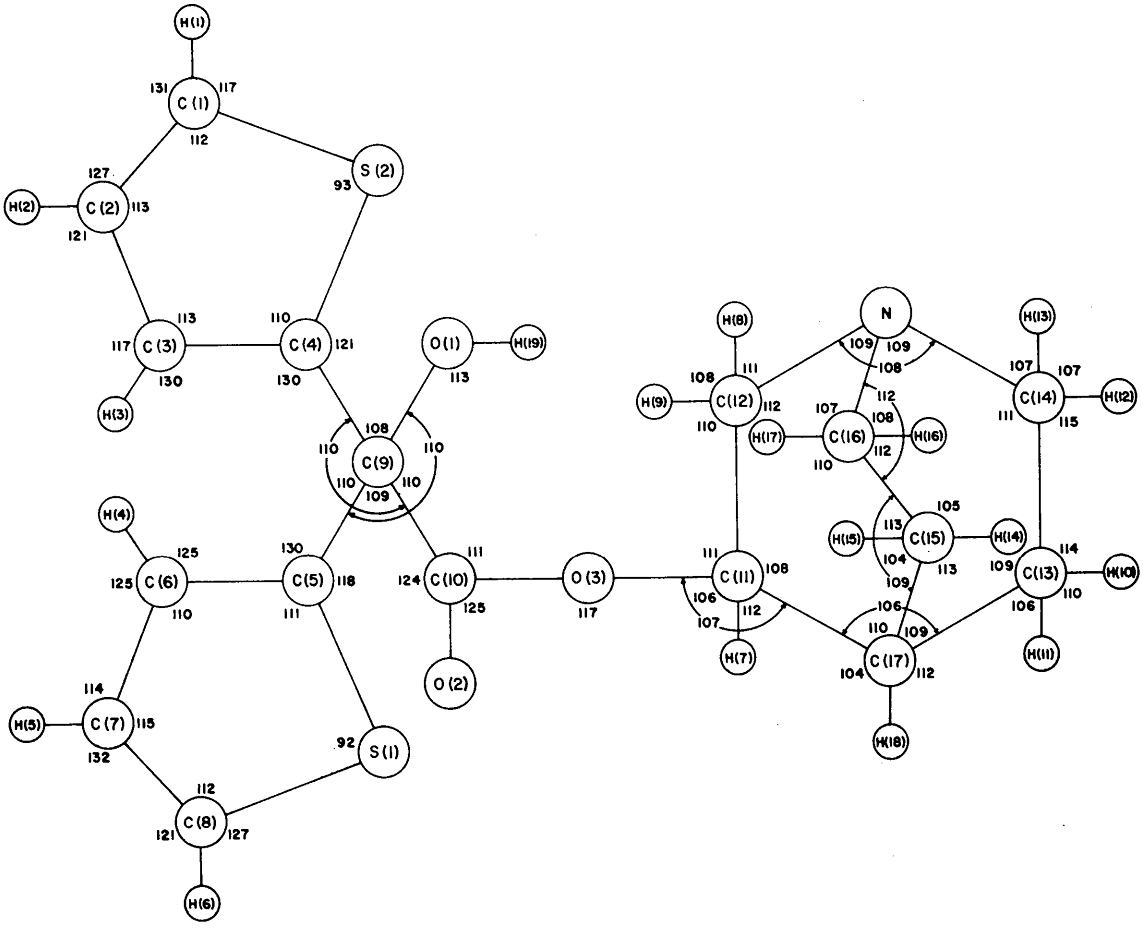

Fig. 4. Bond angles (°).

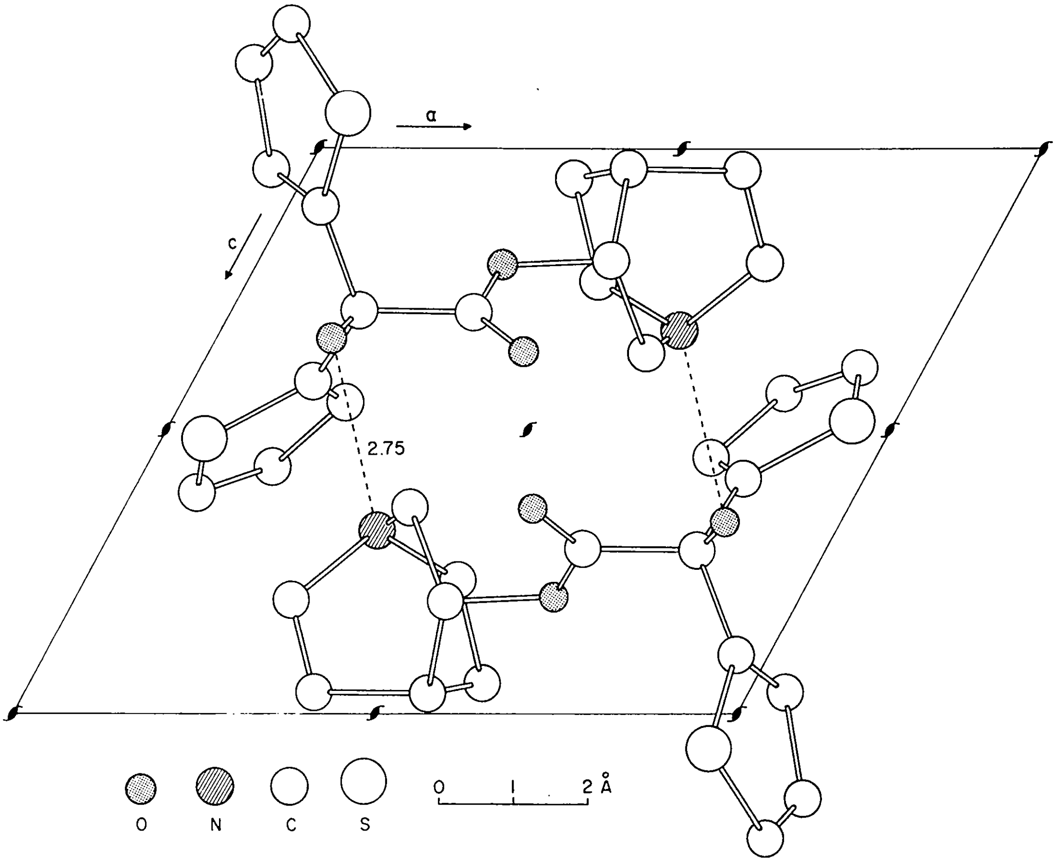

Fig. 5. Quinuclidinyl di-α,α′-thienylglycollate. Projection of the structure along the *b* axis showing intermolecular hydrogen bonds (Å). All hydrogen atoms and adjacent symmetry related molecules are omitted.

Donohue, J. (1950). *J. Amer. Chem. Soc.* **72**, 2701.

Gabel, N. W. & Abood, L. G. (1965). *J. Med. Chem.* **8**, 616.

Hudson, P. & Robertson, J. H. (1962). *Acta Cryst.* **15**, 913.

Hudson, P. & Robertson, J. H. (1964). *Acta Cryst.* **17**, 1497

International Tables for X-ray Crystallography (1962). Vol. III. Birmingham: Kynoch Press.

Johnson, C. K. (1965). *ORTEP, A Fortran Thermal Ellipsoid Plot Program for Crystal Structure Illustrations.* ORNL-3794, Oak Ridge National Laboratory, Tennessee.

Meyerhöffer, A. & Carlström, D. (1969). *Acta Cryst.* B**25**, 1119.

Momany, F. A. (1964). *Dissert. Abstr.* **24**, 2714.

Nardelli, M., Fava, G. & Giraldi, G. (1962). *Acta Cryst.* **15**, 737.

Nyberg, K., Östman, B. & Wallerberg, G. (1970). *Acta Chem. Scand.* In the press.

Pauling, L. (1960). *The Nature of the Chemical Bond*, p. 189. Ithaca: Cornell Univ. Press.

Ringertz, H. (1969). Thesis, Stockholm.

Stewart, J. M. & High, D. (1965). *X-ray* 63, *Program System for X-ray Crystallography* for the IBM 7090. Univ. of Washington, Seattle and Univ. of Maryland. College Park.

Visser, G. J., Heeres, G. J., Wolters, J. & Vos, A. (1968). *Acta Cryst.* B**24**, 467.

Walker, L. A., Folting, K. & Merritt, L. L. Jr (1969). *Acta Cryst.* B**25**, 88.