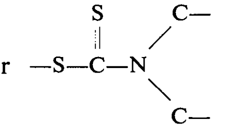
Acta Cryst. (1967). **22**, 273

The Crystal and Molecular Structure of Tetraethylthiuram Disulfide, $C_{10}N_2H_{20}S_4$

By I. L. Karle, J. A. Estlin and K. Britts
U.S. Naval Research Laboratory, Washington, D.C. 20390, *U.S.A.*

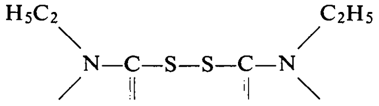
(*Received* 11 *April* 1966 *and in revised form* 29 *July* 1966)

Tetraethylthiuram disulfide (disulfiram, Antabuse) is an antioxidant that interferes with the normal metabolic degradation of alcohol in the body. Whereas the structural formula of this material was well established the configuration was not .The material crystallizes in the monoclinic system, space group $P2_1/c$, with four molecules in the unit cell and the following cell parameters: $a=11\cdot11$, $b=15\cdot90$, $c=8\cdot66$ Å and $\beta=92°42'$. The crystal structure analysis has established that the molecule contains two planar  groups, which are nearly perpendicular to each other; the configuration about each N atom is planar rather than pyramidal. Furthermore, it has been shown that the two C–N bond lengths adjacent to the C=S bonds are both very short, 1·33 and 1·36 Å. Thus there is strong evidence of an influence on the C–N bond length by the C=S bond.

The structure was solved by obtaining the phases directly from the structure factor magnitudes by means of the symbolic addition procedure.

Introduction

Tetraethylthiuram disulfide (disulfiram, Antabuse) (I) has long been known to be of value in the treatment of chronic alcoholism. It prevents the normal degradation of alcohol, resulting in increased acetaldehyde concentrations in blood and tissues. The consumption of only a small quantity of alcohol will produce highly unpleasant reactions in the subject. This substance is also of interest because very few crystal structure analyses have been reported for molecules that contain the S–S bond.



(I)

Experimental

Tetraethylthiuram disulfide was obtained from Bios Laboratories, Inc. Recrystallization from ethyl alcohol at room temperature yielded faintly yellow tabular crystals. The crystal used for data collection had the dimensions 0·2 × 0·3 × 0·2 mm.

The cell parameters, determined from precession photographs using Cu $K\alpha$ radiation, are

$$a=11\cdot11\pm0\cdot02,\ b=15\cdot90\pm0\cdot03,\ c=8\cdot66\pm0\cdot02\ \text{Å}\ ,$$
$$\beta=92°42'\pm15'\ .$$

The unit-cell dimensions, determined from powder data, were reported by Grabar & McCrone (1950) to be $a=13\cdot84$, $b=15\cdot90$, $c=8\cdot66$ Å, and $\beta=126°$. The transformation matrix from their cell to the one used here is:

$$\begin{pmatrix} -1 & 0 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The density computed from the X-ray data with four molecules per unit cell is 1·286 g.cm^{-3}, while that obtained by measuring with a pycnometer is 1·292 g.cm^{-3}. Systematic absences among the reflections indicated that the space group was $P2_1/c$.

Intensity data were collected by the multiple-film, equi-inclination Weissenberg technique. Layers 0 through 11 were recorded along the b axis with controlled exposures and controlled photographic development. Also, the $0kl$ and $1kl$ data were collected along the a axis. Visual estimates were made of the intensities by comparison with a calibrated film strip. These data were processed by a program prepared by H. Norment and S. Brenner of this laboratory. Corrections for Lorentz and polarization factors and spot size were made, but no absorption correction was applied. The computer output yielded the data in the form of structure factors $|F|$ and normalized structure factors $|E|$.

Structure determination

The structure was solved by obtaining the values of the phases directly from the structure factor magnitudes by means of the symbolic addition procedure (see

Table 1. *The assignments for the application of the Σ_2 phase determination formula*

h	k	l	$\|E\|$	Sign
7	5	1	3·37	+
$\bar{9}$	4	1	3·26	+
$\overline{10}$	3	3	2·95	+
6	1	3	2·42	a
11	4	2	2·69	b

Table 2. *Observed and calculated structure factors*

ANTABUSE

H	K	L	F(OBS)	F(CALC)
-14	1	2	11.0	17,1
-13	0	4	20.6	23,8
-13	1	1	16.3	-18,9
-13	1	2	0.0	-2,4
-13	1	3	14.7	-19,3
-13	1	4	5.9	8,9
-13	2	1	16.3	-18,1
-13	2	3	10.6	13,3
-13	2	4	14.7	20,6
-13	3	2	9.4	10,4
-13	3	3	12.2	-15,5
-13	3	4	8.6	11,9
-13	4	2	23.2	25,7
-13	5	1	6.7	-8,0
-13	5	2	4.5	7,6
-13	6	1	4.3	-5,8
-13	6	2	17.2	21,3
-13	7	1	4.7	4,8
-13	7	2	6.6	-7,8
-12	0	2	12.8	-14,3
-12	0	4	8.0	-7,7
-12	0	6	6.4	5,7
-12	1	1	12.0	-11,8
-12	1	2	9.0	-7,4
-12	1	3	10.0	-11,5
-12	1	4	8.9	9,2
-12	1	5	14.7	16,3
-12	1	6	5.8	-2,8
-12	2	1	0.0	1,1
-12	2	2	5.2	6,1
-12	2	3	0.0	-3,7
-12	2	4	9.6	-9,5
-12	2	5	13.6	-18,2
-12	3	1	11.1	-10,5
-12	3	2	6.2	-5,4
-12	3	3	4.8	4,6
-12	3	4	6.6	6,2
-12	3	5	5.7	6,6
-12	3	6	4.5	-7,1
-12	4	1	25.3	-26,9
-12	4	2	8.6	8,9
-12	4	3	8.1	7,5
-12	4	4	9.8	-10,6
-12	4	5	14.3	16,5
-12	5	1	7.8	-6,8
-12	5	2	5.9	-7,0
-12	5	3	14.7	15,3
-12	5	5	5.0	6,0
-12	6	1	7.0	-6,7
-12	6	2	0.0	-3,4
-12	7	1	0.0	-2,2
-12	7	2	0.0	2,2
-12	7	3	17.0	19,5
-12	7	4	2.9	-4,9
-12	8	1	6.1	6,3
-12	8	4	5.0	-6,3
-12	9	2	11.9	11,5
-12	10	1	9.9	-11,7
-11	0	2	0.0	-3,1
-11	0	4	22.2	-23,7
-11	0	6	0.0	7,2
-11	1	1	17.6	19,4
-11	1	2	8.2	-8,4
-11	1	3	0.0	3,5
-11	1	4	0.0	-4,4
-11	1	5	0.0	-3,9
-11	1	6	0.0	8,8
-11	2	1	11.7	10,3
-11	2	2	8.2	-6,2
-11	2	3	5.6	4,1
-11	2	4	6.5	-5,0
-11	2	5	6.9	6,7
-11	2	7	4.5	-1,1
-11	3	1	0.0	3,8
-11	3	2	17.3	-20,0
-11	3	3	11.8	11,5
-11	3	4	9.1	-9,1
-11	3	5	10.2	-13,4
-11	3	6	6.1	6,2
-11	4	1	14.1	13,9
-11	4	2	10.6	-10,2
-11	4	3	5.5	-5,5
-11	4	4	0.0	1,9
-11	4	5	23.1	22,1
-11	5	1	7.9	8,2
-11	5	2	26.9	-30,5
-11	5	3	8.4	8,8
-11	5	4	10.0	-11,5
-11	5	5	0.0	5,3
-11	6	1	6.7	6,0
-11	6	2	11.4	-12,2
-11	6	3	11.5	12,8
-11	6	4	6.7	5,5
-11	6	5	8.1	8,0
-11	6	6	5.0	4,4
-11	7	1	0.0	2,9
-11	7	2	0.0	-1,8
-11	7	3	12.0	12,7
-11	7	4	20.6	-20,8
-11	7	6	4.9	6,0
-11	8	1	13.1	13,8
-11	8	2	12.8	-14,0
-11	8	3	19.7	19,0
-11	8	4	13.4	15,1
-11	9	2	0.0	0,5
-11	9	3	7.2	7,0
-11	9	4	11.1	-13,5
-11	9	5	4.3	-5,2
-11	10	1	13.5	12,2
-11	10	2	7.8	-8,6
-11	10	3	11.1	12,4
-11	11	1	12.8	17,6
-11	11	2	4.3	-5,5
-11	11	3	4.6	-5,5
-10	0	2	14.7	13,3
-10	0	4	16.5	-16,5
-10	0	6	0.0	-1,1
-10	0	8	5.0	-5,8
-10	1	1	7.3	4,8
-10	1	2	24.2	-25,3
-10	1	3	10.4	12,5
-10	1	4	9.3	8,9
-10	1	5	12.5	-11,2
-10	1	6	0.0	1,3
-10	1	7	10.4	9,7
-10	2	1	16.6	15,5
-10	2	2	12.1	9,6
-10	2	3	0.0	-1,4
-10	2	4	0.0	1,3
-10	2	5	16.7	-17,2
-10	2	6	11.2	-11,1
-10	2	7	7.2	5,1
-10	3	1	18.2	16,1
-10	3	2	13.5	-14,3
-10	3	3	27.0	-30,0
-10	3	4	8.2	-9,0
-10	3	5	0.0	3,7
-10	3	6	12.1	14,1
-10	3	7	10.6	10,8
-10	4	1	20.5	21,1
-10	4	2	0.0	3,7
-10	4	3	12.5	-14,3
-10	4	4	15.2	15,8
-10	4	5	8.5	7,7
-10	5	1	13.3	-13,9
-10	5	2	0.0	1,8
-10	5	3	9.2	-10,3
-10	5	4	8.9	-9,0
-10	5	5	0.0	3,5
-10	5	6	14.9	13,8
-10	6	1	13.1	14,6
-10	6	2	9.2	8,5
-10	6	3	0.0	2,6
-10	6	4	3.8	3,4
-10	6	5	9.4	-10,4
-10	6	6	11.9	13,4
-10	7	1	17.2	-17,1
-10	7	2	25.2	-26,8
-10	7	3	11.7	-10,8
-10	7	4	11.1	12,4
-10	7	6	7.0	6,6
-10	8	1	14.6	16,1
-10	8	2	0.0	2,1
-10	8	3	5.2	4,7
-10	8	4	20.7	21,5
-10	8	5	16.0	-17,2
-10	8	6	7.0	7,2
-10	9	1	7.4	-6,8
-10	9	2	0.0	1,0
-10	9	3	22.8	-25,0
-10	9	4	13.8	12,0
-10	9	5	7.0	-5,0
-10	10	1	0.0	2,7
-10	10	2	10.2	9,7
-10	10	3	0.0	2,4
-10	10	4	10.2	9,3
-10	10	6	4.5	7,2
-10	11	1	8.4	-10,0
-10	11	2	0.0	-1,3
-10	11	3	0.0	-4,9
-10	11	4	10.0	12,9
-10	11	5	11.3	-17,8
-9	0	2	35.2	-32,9
-9	0	4	0.0	-4,5
-9	0	6	24.7	-23,8
-9	0	8	8.5	8,9
-9	1	1	10.1	10,2
-9	1	2	0.0	-1,4
-9	1	3	44.1	42,0
-9	1	4	13.5	14,0
-9	1	5	0.0	4,7
-9	1	6	0.0	-4,0
-9	1	7	0.0	-3,7
-9	1	8	6.9	6,6
-9	1	9	0.0	-0,3
-9	2	1	50.0	51,5
-9	2	2	20.7	18,2
-9	2	3	32.1	-32,0
-9	2	4	20.4	-19,6
-9	2	5	15.7	-13,6
-9	2	6	15.8	-13,7
-9	2	7	7.8	8,0
-9	2	8	7.6	2,2
-9	3	1	12.6	-11,2
-9	3	2	14.6	13,3
-9	3	3	0.0	-0,8
-9	3	4	0.0	-1,5
-9	3	5	26.7	26,5
-9	3	6	0.0	0,2
-9	3	7	9.7	-2,3
-9	3	8	8.7	9,3
-9	4	1	20.8	-19,4
-9	4	2	14.7	-14,2
-9	4	3	0.0	-2,5
-9	4	4	11.2	-11,7
-9	4	5	20.4	-21,9
-9	4	6	9.4	-7,8
-9	5	1	14.6	-14,2
-9	5	2	29.1	29,8
-9	5	3	4.2	5,8
-9	5	4	0.0	-2,3
-9	5	5	15.1	14,6
-9	5	6	0.0	4,6
-9	5	7	6.8	6,0
-9	5	8	5.7	4,3
-9	6	1	11.9	-9,7
-9	6	2	26.5	-28,3
-9	6	3	7.2	-9,0
-9	6	4	0.0	0,5
-9	6	5	15.7	-14,7
-9	6	6	0.0	-0,0
-9	7	1	18.5	-16,9
-9	7	2	20.6	24,3
-9	7	3	0.0	-5,6
-9	7	4	21.3	21,4
-9	7	5	5.3	5,0
-9	7	6	0.0	-2,5
-9	7	7	15.2	14,6
-9	8	1	0.0	-3,2
-9	8	2	18.2	18,1
-9	8	3	19.9	-20,6
-9	8	4	17.3	-15,1
-9	8	5	0.0	1,9
-9	8	6	0.0	-1,8
-9	9	1	19.2	-20,1
-9	9	2	11.8	11,3
-9	9	3	13.3	-13,5
-9	9	4	11.0	10,5
-9	9	5	5.8	5,2
-9	9	7	5.2	5,9
-9	10	1	36.3	-39,0
-9	10	2	20.8	20,4
-9	10	3	0.0	1,1
-9	10	4	0.0	-3,3
-9	10	6	4.4	-4,4
-9	11	1	17.3	-11,5
-9	11	2	6.0	5,2
-9	11	3	0.0	-3,0
-9	11	4	3.8	5,6
-9	11	5	0.0	-2,4
-8	0	2	39.8	-32,0
-8	0	4	25.9	26,2
-8	0	6	13.2	11,8
-8	0	8	10.0	7,8
-8	1	1	15.4	13,7
-8	1	2	36.4	32,6
-8	1	3	22.1	21,4
-8	1	4	13.2	-14,4
-8	1	5	15.9	-16,1
-8	1	6	0.0	-0,3
-8	1	7	22.1	-22,8
-8	1	8	0.0	3,3
-8	1	9	6.6	-7,4
-8	2	1	17.8	-16,1
-8	2	2	15.9	-15,1
-8	2	3	0.0	3,9
-8	2	4	10.3	9,1
-8	2	5	17.1	-17,3
-8	2	6	22.0	22,5
-8	2	7	0.0	2,6
-8	2	8	9.0	7,8
-8	2	9	0.0	3,4
-8	3	1	0.0	3,8
-8	3	2	41.2	35,4
-8	3	3	20.7	16,8
-8	3	4	0.0	0,7
-8	3	5	11.3	-11,3
-8	3	6	8.3	-7,3
-8	3	7	10.8	-10,0
-8	3	8	6.8	4,4
-8	3	9	7.7	-8,5
-8	4	1	0.0	-0,7
-8	4	2	12.2	-11,1
-8	4	3	8.3	8,3
-8	4	4	0.0	-4,8
-8	4	5	12.0	-10,8
-8	4	6	20.4	20,6
-8	4	7	7.5	-5,8
-8	4	8	16.9	13,8
-8	4	9	6.5	6,0
-8	5	1	71.4	65,7
-8	5	2	17.4	18,7
-8	5	3	17.7	-16,9
-8	5	4	6.5	8,6
-8	5	5	8.4	-7,4
-8	5	6	9.0	-7,2
-8	5	7	7.2	-6,7
-8	5	8	0.0	-1,6
-8	6	1	9.1	-7,8
-8	6	2	12.3	-10,6
-8	6	3	9.3	-9,0
-8	6	4	24.1	-21,9
-8	6	5	0.0	2,7
-8	6	6	10.4	8,3
-8	6	8	10.7	10,9
-8	7	1	44.2	43,3
-8	7	2	5.8	7,1
-8	7	3	11.0	-10,0
-8	7	4	0.0	-1,2
-8	7	5	7.0	-5,1
-8	7	6	8.4	7,1
-8	7	7	0.0	-0,0
-8	7	8	0.0	-3,8
-8	8	1	18.2	-18,8
-8	8	2	7.1	-5,3
-8	8	3	21.8	-20,2
-8	8	4	9.9	-9,2
-8	8	5	18.9	17,9
-8	8	6	0.0	-1,2
-8	8	8	0.0	5,1
-8	9	1	22.1	-21,2
-8	9	2	20.0	-20,8
-8	9	3	27.3	25,9
-8	9	4	5.5	-5,4
-8	9	5	6.4	-5,3
-8	9	7	3.3	5,0
-8	9	8	0.0	0,8
-8	10	1	8.7	-6,2
-8	10	2	15.6	-14,0
-8	10	3	6.6	5,3
-8	10	4	0.0	-0,6
-8	10	5	11.0	9,6
-8	10	6	0.0	-0,3
-8	10	7	6.5	6,2
-8	11	1	0.0	2,8
-8	11	2	14.0	-14,3
-8	11	3	7.3	7,6
-8	11	4	0.0	-1,0
-8	11	5	7.1	6,7
-8	11	6	6.6	-5,4
-8	11	7	5.1	-5,7
-7	0	2	24.2	26,8
-7	0	4	43.7	42,2
-7	0	6	29.4	31,1
-7	0	8	16.8	-16,4
-7	1	1	45.5	-41,5
-7	1	2	10.2	-7,4
-7	1	3	50.4	-49,6
-7	1	4	19.7	17,7
-7	1	5	0.0	-3,7
-7	1	6	8.5	-7,5
-7	1	7	0.0	-1,3
-7	1	8	0.0	-1,0
-7	1	9	0.0	4,9
-7	2	1	49.0	-44,3
-7	2	2	14.7	8,8
-7	2	3	32.6	28,2
-7	2	4	40.4	40,5
-7	2	5	8.4	-7,7
-7	2	6	12.1	8,8
-7	2	7	0.0	-1,9
-7	2	8	11.6	-10,1
-7	2	9	0.0	0,3
-7	3	1	15.5	-15,0
-7	3	2	10.5	-9,1
-7	3	3	48.5	-45,5
-7	3	4	24.6	22,4
-7	3	5	11.2	-10,3
-7	3	6	12.8	-12,5
-7	3	7	0.0	-2,6
-7	3	8	0.0	-2,1
-7	3	9	10.3	9,8
-7	4	1	29.6	-27,4
-7	4	2	14.2	10,4
-7	4	3	14.7	14,1
-7	4	4	42.5	42,4
-7	4	5	7.3	5,4
-7	4	6	0.0	-3,4
-7	4	7	10.6	-9,4
-7	4	8	3.5	-4,5
-7	4	9	11.3	12,4
-7	5	1	11.2	-10,8
-7	5	2	42.4	40,0
-7	5	3	0.0	2,7
-7	5	4	10.1	7,7
-7	5	5	29.1	-32,6
-7	5	6	8.4	-8,3
-7	5	7	11.8	12,1
-7	5	8	7.5	-8,6
-7	5	9	9.1	10,1
-7	6	1	10.1	-7,8
-7	6	2	45.1	40,9
-7	6	3	0.0	-0,3
-7	6	4	11.0	-10,4
-7	6	5	7.3	-6,5
-7	6	6	0.0	-1,1
-7	6	7	5.3	4,4
-7	6	8	0.0	-3,0
-7	7	1	14.5	14,6
-7	7	2	11.1	-8,6
-7	7	3	9.0	-5,8
-7	7	4	5.8	5,3
-7	7	5	7.2	-5,6
-7	7	6	0.0	2,0
-7	7	7	8.1	7,3
-7	7	8	0.0	-1,3
-7	7	9	7.9	8,6
-7	8	1	0.0	-0,8
-7	8	2	22.8	17,9
-7	8	3	0.0	2,8
-7	8	4	8.2	-8,4
-7	8	5	8.1	-7,7
-7	8	6	6.7	-7,3
-7	8	7	0.0	-1,5
-7	8	8	0.0	-2,6
-7	9	1	27.5	24,6
-7	9	2	7.9	-7,8
-7	9	3	10.6	-9,8
-7	9	4	6.9	-7,1
-7	9	5	3.9	0,1
-7	9	6	13.7	14,6
-7	9	7	6.7	4,6
-7	9	8	0.0	1,9
-7	10	1	22.5	20,7
-7	10	2	11.0	-11,3
-7	10	3	19.2	-15,8
-7	10	4	0.0	2,0
-7	10	5	0.0	3,8
-7	10	6	4.8	-3,9
-7	10	7	0.0	-1,7
-7	10	8	10.7	-11,7
-7	11	1	0.0	5,2
-7	11	2	10.0	-8,9
-7	11	3	11.3	10,4
-7	11	4	0.0	0,1
-7	11	5	9.2	7,6
-7	11	6	5.4	3,8
-7	11	7	0.0	0,7
-6	0	2	22.4	-18,7
-6	0	4	21.7	-24,8
-6	0	6	20.5	-19,0
-6	0	8	0.0	1,1
-6	1	1	61.5	-52,7
-6	1	2	8.7	-9,6
-6	1	3	18.4	-20,0
-6	1	4	5.3	4,7
-6	1	5	21.1	19,8
-6	1	6	5.9	5,1
-6	1	7	19.3	22,0
-6	1	8	5.5	-2,4
-6	1	9	0.0	-3,4
-6	2	1	11.1	-9,3
-6	2	2	40.9	38,7
-6	2	3	11.2	7,3
-6	2	4	21.6	-18,6
-6	2	5	23.1	23,3
-6	2	6	7.3	-6,4
-6	2	7	0.0	0,3
-6	2	8	8.7	-8,1
-6	2	9	0.0	-0,5
-6	3	1	16.0	-12,2
-6	3	2	25.2	-22,8
-6	3	3	11.4	-8,9
-6	3	4	6.6	4,8
-6	3	5	22.3	22,9
-6	3	6	7.3	-6,9
-6	3	7	7.3	6,8
-6	3	8	14.5	-13,8
-6	3	9	0.0	3,8
-6	4	1	65.1	-58,0
-6	4	2	35.9	34,2
-6	4	3	27.4	26,7
-6	4	4	11.7	-10,4
-6	4	5	11.7	12,3
-6	4	6	22.5	-20,9
-6	4	7	13.2	11,0
-6	4	8	7.6	-5,3
-6	4	9	0.0	2,8
-6	5	1	18.9	-17,2
-6	5	2	6.1	-6,1
-6	5	3	26.4	24,1
-6	5	4	10.4	-9,2
-6	5	5	0.0	0,6
-6	5	6	15.9	-16,5
-6	5	7	14.2	14,3
-6	5	8	14.7	-15,6
-6	5	9	0.0	-2,9
-6	6	1	9.3	7,1
-6	6	2	10.8	-11,3
-6	6	3	23.9	-21,4
-6	6	4	0.0	-3,1
-6	6	5	27.1	28,9
-6	6	6	27.4	-28,4
-6	6	7	8.0	10,3
-6	6	8	7.1	6,8
-6	7	1	40.8	-34,6
-6	7	2	0.0	-2,1
-6	7	3	40.7	38,4
-6	7	4	6.9	4,7
-6	7	5	13.1	11,6
-6	7	6	17.2	-18,3
-6	7	7	0.0	-4,3
-6	7	8	0.0	-1,5
-6	7	9	0.0	-1,0
-6	8	1	31.6	24,2
-6	8	2	26.4	22,8
-6	8	3	12.3	-10,9
-6	8	4	27.6	-25,3
-6	8	5	10.8	9,2
-6	8	6	13.9	-13,6
-6	8	7	11.1	11,6
-6	8	8	0.0	3,2
-6	8	9	7.8	8,5
-6	9	1	0.0	-0,8
-6	9	2	13.1	10,0
-6	9	3	28.8	28,7
-6	9	4	16.0	-16,6
-6	9	5	9.0	7,9
-6	9	6	5.4	4,1
-6	9	7	0.0	-1,0
-6	9	8	7.7	-6,1
-6	10	1	7.4	-5,3
-6	10	2	14.2	-10,4
-6	10	3	0.0	0,6
-6	10	4	6.8	6,0
-6	10	5	23.2	-21,2
-6	10	6	8.1	-6,1
-6	10	7	15.7	15,6
-6	10	8	4.3	-1,0
-6	11	1	18.1	18,0
-6	11	2	45.2	46,8
-6	11	3	0.0	-0,4
-6	11	4	16.7	-16,0
-6	11	5	10.4	8,8
-6	11	6	4.8	-3,3
-6	11	7	3.5	2,2
-6	11	8	4.3	-4,7
-5	0	2	10.0	16,4
-5	0	4	74.2	-75,1
-5	0	6	21.4	20,8
-5	0	8	0.0	5,7
-5	0	10	5.6	-5,6
-5	1	1	81.8	81,4
-5	1	2	10.2	-8,3
-5	1	3	13.6	-12,2
-5	1	4	26.0	-26,4
-5	1	5	17.1	18,8
-5	1	6	14.3	13,0
-5	1	7	0.0	-1,0
-5	1	8	8.2	-6,4
-5	1	9	0.0	-2,4
-5	2	1	0.0	1,7
-5	2	2	37.6	-39,0
-5	2	3	9.2	4,6
-5	2	4	35.6	-33,3
-5	2	5	25.1	26,3
-5	2	6	14.4	12,3
-5	2	7	11.3	-11,5
-5	2	8	5.8	5,1
-5	2	9	0.0	-3,4
-5	3	1	4.1	1,5
-5	3	2	74.8	-75,0
-5	3	3	43.2	42,4
-5	3	4	0.0	1,9
-5	3	5	22.8	-22,4
-5	3	6	5.9	4,6
-5	3	7	0.0	2,3
-5	3	8	4.0	-4,3
-5	3	9	0.0	-1,4
-5	4	1	44.1	39,4
-5	4	2	25.8	-21,9
-5	4	3	0.0	-1,4
-5	4	4	9.7	8,4
-5	4	5	38.3	37,4
-5	4	6	5.9	-5,4
-5	4	7	8.5	7,0
-5	4	8	8.0	6,3
-5	4	9	6.7	-8,6
-5	5	1	21.9	18,4
-5	5	2	57.3	-55,4
-5	5	3	28.4	23,8
-5	5	4	26.5	-26,1
-5	5	5	0.0	1,2
-5	5	6	8.4	-7,7
-5	5	7	15.8	-15,2
-5	5	8	6.7	6,3
-5	5	9	11.2	-8,8
-5	5	10	7.2	7,2
-5	6	1	24.3	21,5
-5	6	2	46.7	-47,0
-5	6	3	10.6	10,0
-5	6	4	19.6	18,2
-5	6	5	29.0	31,5
-5	6	6	0.0	2,3
-5	6	7	0.0	0,2
-5	6	8	11.3	10,9
-5	6	9	11.2	-9,5
-5	7	1	0.0	4,2
-5	7	2	0.0	-0,5
-5	7	3	24.6	23,3
-5	7	4	44.8	-47,9
-5	7	5	12.2	12,1
-5	7	6	0.0	-1,3
-5	7	7	33.2	-35,5
-5	7	8	6.2	5,9
-5	7	9	0.0	-2,0
-5	8	1	8.8	7,0
-5	8	2	38.0	-35,1
-5	8	3	46.2	48,6
-5	8	4	15.6	13,0
-5	8	5	5.7	-6,5
-5	8	6	26.8	25,9
-5	8	7	0.0	1,4
-5	8	8	4.8	4,2
-5	8	9	5.4	-5,3
-5	9	1	0.0	3,6
-5	9	2	15.4	-15,9
-5	9	3	9.1	4,4
-5	9	4	3.9	-4,6
-5	9	5	17.7	-11,7
-5	9	6	15.9	-16,5
-5	9	7	11.7	-12,0
-5	9	8	0.0	2,8
-5	9	9	7.1	-7,4
-5	10	1	0.0	2,2
-5	10	2	8.0	-6,4
-5	10	3	31.3	31,9
-5	10	4	5.4	5,4
-5	10	5	0.0	3,5
-5	10	6	14.2	13,4
-5	10	7	0.0	1,1
-5	10	8	8.5	9,1
-5	11	1	44.4	42,8
-5	11	2	0.0	0,2
-5	11	3	19.5	-19,7
-5	11	4	0.0	0,2
-5	11	5	6.5	-6,4
-5	11	6	15.2	-14,5
-5	11	7	9.4	-11,1
-5	11	8	9.0	9,4
-4	0	2	63.5	63,3
-4	0	4	26.2	-23,2
-4	0	6	11.9	-9,7
-4	0	8	0.0	-0,2
-4	0	10	6.2	-5,6
-4	1	1	0.0	-0,9
-4	1	2	9.2	7,1
-4	1	3	39.5	40,0
-4	1	4	10.3	-6,7
-4	1	5	24.7	-24,9
-4	1	6	21.0	21,5
-4	1	7	18.0	17,8
-4	1	8	0.0	-0,6
-4	1	9	11.9	10,4
-4	2	1	52.4	53,0
-4	2	2	6.6	-4,1
-4	2	3	15.7	13,3
-4	2	4	23.5	-21,7
-4	2	5	23.1	-21,2
-4	2	6	26.5	27,0
-4	2	7	7.3	-7,1
-4	2	8	0.0	-1,3
-4	2	9	12.9	-13,0
-4	2	10	7.8	8,5
-4	3	1	34.7	31,1
-4	3	2	12.6	5,3
-4	3	3	25.9	-18,9
-4	3	4	39.9	-37,8
-4	3	5	11.8	-10,4
-4	3	6	33.1	34,2
-4	3	7	0.0	0,3
-4	3	8	7.2	7,3
-4	3	9	14.7	11,4
-4	4	1	72.4	68,6
-4	4	2	9.9	3,4
-4	4	3	42.1	-38,2
-4	4	4	28.3	27,8
-4	4	5	20.8	-21,1
-4	4	6	0.0	-0,8
-4	4	7	0.0	0,4
-4	4	8	14.2	-14,5
-4	4	9	10.1	-9,8
-4	5	1	42.3	-42,3
-4	5	2	5.9	-5,5
-4	5	3	35.4	-34,1
-4	5	4	24.3	-23,4
-4	5	5	15.5	14,2
-4	5	6	26.3	26,1
-4	5	7	0.0	-0,9
-4	5	8	17.1	17,9
-4	5	9	0.0	3,4
-4	6	1	33.8	28,2
-4	6	2	10.5	6,4
-4	6	3	13.3	11,0
-4	6	4	22.7	20,2
-4	6	5	17.4	-17,8
-4	6	6	23.8	24,7
-4	6	7	19.3	-18,9
-4	6	8	16.7	-17,8
-4	6	9	7.0	-4,7
-4	7	1	34.9	-32,1
-4	7	2	39.5	-37,8
-4	7	3	37.3	-34,3
-4	7	4	27.4	25,3
-4	7	5	0.0	-0,3
-4	7	6	7.1	5,3
-4	7	7	0.0	-4,2
-4	7	8	22.3	22,3
-4	7	9	8.5	8,3
-4	8	1	30.2	28,1
-4	8	2	5.5	-2,7
-4	8	3	43.4	44,4
-4	8	4	37.1	36,4
-4	8	5	28.0	-29,9
-4	8	6	21.8	19,5
-4	8	7	16.7	-16,0
-4	8	8	10.1	-10,1
-4	8	9	6.9	-6,0
-4	9	1	16.5	15,0
-4	9	2	11.4	-8,3
-4	9	3	45.4	-50,8
-4	9	4	31.1	29,9
-4	9	5	20.3	-20,8
-4	9	6	0.0	2,8
-4	9	7	0.0	0,2
-4	9	8	5.8	6,1
-4	9	9	0.0	2,7
-4	10	1	26.3	22,3
-4	10	2	40.4	43,3
-4	10	3	15.7	-13,0
-4	10	4	20.3	22,4
-4	10	5	3.9	1,1
-4	10	6	0.0	1,4
-4	10	7	18.2	-18,1
-4	10	8	0.0	2,7
-4	10	9	3.6	4,3
-4	11	1	31.7	-27,6
-4	11	2	0.0	-2,3
-4	11	3	14.3	-15,1
-4	11	4	7.5	-6,7
-4	11	5	16.6	-19,1
-4	11	6	11.1	10,9
-4	11	7	4.7	4,4
-4	11	8	0.0	0,6
-3	0	2	16.4	-24,8
-3	0	4	6.0	-5,1
-3	0	6	60.1	-58,8
-3	0	8	10.3	8,3
-3	0	10	24.5	21,6
-3	1	1	22.8	14,0
-3	1	2	7.5	-2,7
-3	1	3	36.4	37,7
-3	1	4	0.0	-2,7
-3	1	5	30.6	29,8
-3	1	6	6.7	-6,1
-3	1	7	10.2	-9,2
-3	1	8	16.9	17,1
-3	1	9	6.7	-6,1
-3	2	1	50.5	51,2
-3	2	2	6.9	2,5
-3	2	3	30.1	-34,2
-3	2	4	11.7	-12,5
-3	2	5	20.1	-19,2
-3	2	6	13.6	-13,1
-3	2	7	14.6	-11,6
-3	2	8	0.0	3,3
-3	2	9	8.6	6,8
-3	2	10	11.2	10,6
-3	3	1	8.8	8,1
-3	3	2	77.9	79,8
-3	3	3	20.9	16,0
-3	3	4	9.6	11,0
-3	3	5	17.5	16,1
-3	3	6	7.9	-3,5
-3	3	7	7.3	6,4
-3	3	8	13.3	12,8
-3	3	9	0.0	-0,4
-3	4	1	29.5	-25,0
-3	4	2	22.5	26,7
-3	4	3	16.6	-15,3
-3	4	4	67.6	-63,3
-3	4	5	53.5	-52,8
-3	4	6	0.0	5,5
-3	4	7	15.9	14,3
-3	4	8	0.0	-0,8
-3	4	9	0.0	0,0
-3	4	10	7.8	7,2
-3	5	1	26.3	-23,5
-3	5	2	23.4	22,5
-3	5	3	5.9	-5,5
-3	5	4	30.4	32,6
-3	5	5	16.7	16,8
-3	5	6	19.7	18,8
-3	5	7	25.2	24,6
-3	5	8	0.0	-0,3
-3	5	9	18.1	-18,6
-3	6	1	15.9	-14,0
-3	6	2	16.3	-14,6
-3	6	3	36.4	-36,0
-3	6	4	15.2	-11,4
-3	6	5	20.8	-18,5
-3	6	6	16.4	-14,7
-3	6	7	10.3	-9,3
-3	6	8	0.0	-2,2
-3	6	9	6.9	7,2
-3	7	1	28.4	-26,8
-3	7	2	11.4	8,7
-3	7	3	13.7	-14,3
-3	7	4	37.9	36,2
-3	7	5	10.9	9,2
-3	7	6	12.9	12,4
-3	7	7	26.2	24,9
-3	7	8	0.0	-2,6
-3	7	9	8.9	-7,1
-3	8	1	17.8	-14,7

Table 2 (*cont.*)

-3	8	2	31.4	26.8
-3	8	3	44.5	-47.7
-3	8	4	16.5	-15.4
-3	8	5	0.0	-3.4
-3	8	6	0.0	-0.7
-3	8	7	8.1	-7.6
-3	8	8	9.8	-11.1
-3	8	9	0.0	0.8
-3	9	1	24.8	-22.6
-3	9	2	17.4	16.6
-3	9	3	25.5	-25.6
-3	9	4	25.0	24.4
-3	9	5	19.4	19.4
-3	9	6	0.0	2.6
-3	9	7	6.7	7.5
-3	9	8	12.1	-12.0
-3	9	9	9.5	9.1
-3	10	1	39.1	-39.7
-3	10	2	34.7	37.4
-3	10	3	18.8	-18.1
-3	10	4	10.3	-9.4
-3	10	5	3.8	3.9
-3	10	6	11.1	-9.4
-3	10	7	0.0	1.1
-3	10	8	0.0	0.5
-3	10	9	5.0	4.6
-3	11	1	44.0	-44.3
-3	11	2	15.5	14.9
-3	11	3	3.4	2.3
-3	11	4	11.0	12.1
-3	11	5	0.0	0.0
-3	11	6	7.5	6.9
-3	11	7	6.0	5.6
-3	11	8	15.9	-16.5
-3	11	9	3.9	4.5
-2	0	2	8.2	-6.9
-2	0	4	47.2	44.0
-2	0	6	25.9	24.7
-2	0	8	27.2	25.9
-2	0	10	12.5	10.1
-2	1	1	52.6	53.7
-2	1	2	56.0	47.9
-2	1	3	13.6	5.4
-2	1	4	34.2	-31.7
-2	1	5	16.6	14.4
-2	1	6	7.6	5.1
-2	1	7	43.1	-44.8
-2	1	8	0.0	-2.3
-2	1	9	15.8	-15.9
-2	2	1	23.3	-27.3
-2	2	2	98.5	-100.7
-2	2	3	28.1	23.1
-2	2	4	26.3	25.2
-2	2	5	6.8	-6.0
-2	2	6	31.2	29.4
-2	2	7	21.9	-21.2
-2	2	8	12.8	12.9
-2	2	9	12.4	12.5
-2	2	10	7.8	7.2
-2	3	1	24.8	-19.7
-2	3	2	70.5	68.8
-2	3	3	40.6	42.5
-2	3	4	9.6	6.7
-2	3	5	51.8	-51.2
-2	3	6	12.3	-12.1
-2	3	7	17.8	-17.2
-2	3	8	0.0	1.1
-2	3	9	7.8	-7.0
-2	4	1	42.3	-45.0
-2	4	2	46.6	-48.9
-2	4	3	33.1	-22.5
-2	4	4	10.8	-10.2
-2	4	5	0.0	-7.0
-2	4	6	32.9	35.3
-2	4	7	12.6	11.9
-2	4	8	12.6	11.3
-2	4	9	6.6	5.0
-2	4	10	0.0	2.0
-2	5	1	51.3	53.9
-2	5	2	19.4	22.7
-2	5	3	10.5	5.7
-2	5	4	54.2	55.4
-2	5	5	14.5	13.3
-2	5	6	35.0	-35.0
-2	5	7	23.3	-23.5
-2	5	8	0.0	0.9
-2	5	9	0.0	-3.0
-2	6	1	50.8	-50.4
-2	6	2	11.6	10.3
-2	6	3	9.1	7.2
-2	6	4	27.5	-29.4
-2	6	5	11.0	-7.3
-2	6	6	0.0	0.4
-2	6	7	0.0	0.6
-2	6	8	20.2	21.6
-2	6	9	7.1	7.7
-2	7	1	55.2	63.2
-2	7	2	41.6	40.5
-2	7	3	16.8	16.5
-2	7	4	19.9	-19.1
-2	7	5	0.0	-1.4
-2	7	6	9.9	7.0
-2	7	7	0.0	5.7
-2	7	8	7.9	-7.5
-2	7	9	3.3	-4.5
-2	8	1	25.7	-28.0
-2	8	2	28.9	-29.8
-2	8	3	0.0	-2.1
-2	8	4	13.8	-11.9
-2	8	5	8.5	8.4
-2	8	6	7.0	-6.2
-2	8	7	0.0	1.0
-2	8	8	3.8	3.9
-2	8	9	3.8	-3.8
-2	9	1	8.7	7.8
-2	9	2	6.3	3.9
-2	9	3	14.6	14.8
-2	9	4	9.9	-8.7
-2	9	5	12.1	-11.1
-2	9	6	10.6	-8.7
-2	9	7	11.2	9.6
-2	9	8	0.0	1.3
-2	9	9	0.0	2.1
-2	10	1	23.2	-24.3
-2	10	2	28.5	-30.3
-2	10	3	12.1	-10.6
-2	10	4	22.7	-20.9
-2	10	5	25.3	27.9
-2	10	6	6.8	-6.9
-2	10	7	11.9	11.6
-2	10	8	0.0	3.7
-2	10	9	6.9	-7.4
-2	11	1	0.0	-0.5
-2	11	2	26.4	-26.9
-2	11	3	21.8	22.2
-2	11	4	6.2	-6.5
-2	11	5	16.0	16.5
-2	11	6	5.3	-3.6
-2	11	7	3.5	-4.0
-2	11	8	0.0	-1.5
-2	11	9	2.5	3.4
-1	0	2	76.2	83.4
-1	0	4	20.6	15.8
-1	0	6	42.2	38.3
-1	0	8	11.2	-12.0
-1	0	10	13.9	-12.7
-1	1	1	117.9	-124.6
-1	1	2	63.4	-62.4
-1	1	3	58.6	-55.9
-1	1	4	16.1	19.8
-1	1	5	36.0	-34.3
-1	1	6	6.5	4.8
-1	1	7	0.0	-4.3
-1	1	8	0.0	1.4
-1	1	9	6.9	7.8
-1	2	1	5.0	-11.1
-1	2	2	56.8	55.6
-1	2	3	44.6	45.0
-1	2	4	76.7	84.0
-1	2	5	13.5	-9.8
-1	2	6	17.3	14.5
-1	2	7	0.0	0.6
-1	2	8	12.8	-10.9
-1	2	9	9.7	10.2
-1	2	10	14.3	-13.7
-1	3	1	41.9	49.9
-1	3	2	41.2	43.0
-1	3	3	73.0	-78.8
-1	3	4	17.9	-17.0
-1	3	5	35.8	-36.7
-1	3	6	10.9	-9.8
-1	3	7	14.5	14.7
-1	3	8	10.4	-8.4
-1	3	9	9.6	6.9
-1	4	1	0.0	1.9
-1	4	2	14.2	18.8
-1	4	3	38.8	-35.7
-1	4	4	52.8	49.8
-1	4	5	45.4	42.0
-1	4	6	19.8	20.2
-1	4	7	12.6	-11.9
-1	4	8	10.4	-7.7
-1	4	9	5.4	3.9
-1	4	10	14.0	-12.4
-1	5	1	7.4	-8.4
-1	5	2	46.0	45.7
-1	5	3	18.5	-16.9
-1	5	4	19.8	16.5
-1	5	5	24.4	-28.7
-1	5	6	17.3	-16.8
-1	5	7	0.0	-1.4
-1	5	8	18.8	-18.0
-1	5	9	15.0	15.9
-1	6	1	32.3	-32.8
-1	6	2	70.4	77.4
-1	6	3	29.4	21.8
-1	6	4	34.7	-29.9
-1	6	5	0.0	-0.8
-1	6	6	0.0	-3.0
-1	6	7	8.4	8.5
-1	6	8	0.0	-2.7
-1	6	9	0.0	2.0
-1	7	1	12.9	13.8
-1	7	2	54.2	-56.9
-1	7	3	13.7	10.8
-1	7	4	7.3	-5.9
-1	7	5	23.3	-22.3
-1	7	6	16.1	15.5
-1	7	7	5.9	6.3
-1	7	8	6.9	-9.0
-1	7	9	9.1	8.5
-1	8	1	12.7	10.9
-1	8	2	8.8	-5.6
-1	8	3	11.1	11.9
-1	8	4	25.4	25.9
-1	8	5	11.9	-10.4
-1	8	6	26.3	-28.0
-1	8	7	10.8	11.7
-1	8	8	0.0	1.2
-1	8	9	0.0	-2.6
-1	9	1	44.8	53.5
-1	9	2	6.5	-5.7
-1	9	3	3.0	-3.0
-1	9	4	23.0	-23.9
-1	9	5	7.6	9.6
-1	9	6	12.6	13.0
-1	9	7	0.0	0.0
-1	9	8	8.9	8.7
-1	9	9	10.8	9.4
-1	10	1	42.3	50.4
-1	10	2	17.4	-17.3
-1	10	3	26.2	-27.6
-1	10	4	7.0	4.1
-1	10	5	0.0	1.3
-1	10	6	0.0	-0.8
-1	10	7	7.6	-7.1
-1	10	8	8.2	-8.6
-1	10	9	0.0	-1.2
-1	11	1	14.5	-14.5
-1	11	2	2.8	-2.0
-1	11	3	17.2	19.0
-1	11	4	10.5	-9.0
-1	11	5	10.6	8.8
-1	11	6	6.5	6.7
-1	11	7	6.2	5.8
-1	11	8	9.2	8.1
-1	11	9	0.0	1.7
0	0	2	85.3	-93.0
0	0	4	0.0	-7.5
0	0	6	38.7	-35.6
0	0	8	12.7	-13.4
0	1	1	56.2	-61.9
0	1	2	140.2	-135.4
0	1	3	48.0	-49.0
0	1	4	26.1	27.3
0	1	5	35.0	33.5
0	1	6	17.1	-15.8
0	1	7	29.0	30.6
0	1	8	0.0	-0.7
0	1	9	0.0	1.0
0	2	1	19.1	-13.9
0	2	2	40.7	45.4
0	2	3	2.4	-1.6
0	2	4	19.5	-16.6
0	2	5	19.0	19.7
0	2	6	15.2	-11.6
0	2	7	0.0	-2.5
0	2	8	17.1	-15.3
0	2	9	3.9	3.8
0	2	10	0.0	-1.1
0	3	1	46.6	-54.1
0	3	2	49.6	-52.2
0	3	3	63.4	-60.9
0	3	4	23.4	18.1
0	3	5	36.4	35.2
0	3	6	15.4	-11.6
0	3	7	21.7	20.7
0	3	8	17.0	-17.2
0	3	9	5.5	5.8
0	4	1	115.9	-129.8
0	4	2	70.4	79.8
0	4	3	47.6	52.0
0	4	4	25.2	-20.2
0	4	5	44.3	40.2
0	4	6	26.9	-25.0
0	4	7	16.8	14.9
0	4	8	13.4	-12.9
0	4	9	0.0	-0.4
0	4	10	6.5	5.6
0	5	1	60.6	-66.9
0	5	2	6.2	5.7
0	5	3	54.0	49.6
0	5	4	13.9	-10.6
0	5	5	11.2	10.8
0	5	6	13.7	-13.5
0	5	7	0.0	3.5
0	5	8	18.3	-16.6
0	5	9	0.0	4.7
0	6	1	0.0	-1.2
0	6	2	22.3	17.5
0	6	3	15.7	12.6
0	6	4	10.1	-11.3
0	6	5	11.4	11.0
0	6	6	25.1	-24.4
0	6	7	17.0	19.3
0	6	8	0.0	-1.7
0	6	9	0.0	3.6
0	6	10	8.7	6.8
0	7	1	12.5	-19.1
0	7	2	21.9	-19.3
0	7	3	42.9	40.3
0	7	4	13.1	-7.8
0	7	5	11.6	8.6
0	7	6	17.0	-18.1
0	7	7	4.1	3.6
0	7	8	9.8	-6.9
0	7	9	8.4	-7.0
0	7	10	7.9	-6.1
0	8	1	48.5	51.8
0	8	2	8.6	7.4
0	8	3	37.6	-36.2
0	8	4	12.6	-11.7
0	8	5	9.1	10.9
0	8	6	12.7	-12.2
0	8	7	9.1	7.8
0	8	8	0.0	1.4
0	8	9	13.6	10.2
0	8	10	12.5	13.5
0	9	1	0.0	4.6
0	9	2	16.9	16.5
0	9	3	0.0	0.1
0	9	4	12.8	-11.7
0	9	5	23.8	24.4
0	9	6	6.0	-6.0
0	9	7	9.7	-7.6
0	9	8	0.0	-3.0
0	9	9	6.2	-6.5
0	10	1	21.8	-24.0
0	10	2	29.1	-31.5
0	10	3	13.1	10.6
0	10	4	6.0	-5.8
0	10	5	15.5	-14.9
0	10	6	3.9	3.9
0	10	7	10.1	8.4
0	10	8	0.0	2.5
0	10	9	11.0	11.5
0	11	1	13.7	13.4
0	11	2	31.3	-33.1
0	11	3	12.7	14.4
0	11	4	21.6	22.0
0	11	5	7.5	-6.2
0	11	6	3.6	-2.2
0	11	7	0.0	3.2
0	11	8	6.5	-5.9
0	11	9	12.0	-14.7
1	0	2	41.8	-37.1
1	0	4	86.9	-92.6
1	0	6	0.0	-3.1
1	0	8	15.8	16.9
1	0	10	12.5	-3.7
1	1	1	74.9	91.2
1	1	2	0.0	0.0
1	1	3	46.2	44.3
1	1	4	15.8	-10.0
1	1	5	0.0	3.6
1	1	6	17.2	15.3
1	1	7	10.9	9.9
1	1	8	6.0	-4.3
1	1	9	3.9	4.3
1	2	1	88.8	99.1
1	2	2	5.4	1.6
1	2	3	33.5	-30.2
1	2	4	58.4	-60.4
1	2	5	40.6	39.7
1	2	6	7.6	-6.4
1	2	7	7.2	6.5
1	2	8	0.0	4.1
1	2	9	11.1	-10.3
1	2	10	0.0	2.2
1	3	0	37.0	45.5
1	3	1	12.5	8.6
1	3	2	91.3	-94.0
1	3	3	66.8	64.2
1	3	4	26.8	-28.2
1	3	5	0.0	2.3
1	3	6	11.6	8.7
1	3	7	4.2	-5.3
1	3	8	4.2	5.2
1	3	9	11.7	-10.6
1	4	0	21.3	-17.1
1	4	1	61.6	65.3
1	4	2	63.9	-66.8
1	4	3	21.1	-22.4
1	4	4	23.9	22.1
1	4	5	36.3	34.2
1	4	6	11.1	-7.6
1	4	7	0.0	-1.0
1	4	8	9.4	7.4
1	4	9	10.1	-9.1
1	4	10	0.0	1.4
1	5	0	42.6	51.3
1	5	1	3.7	-1.8
1	5	2	47.5	-54.4
1	5	3	31.6	26.6
1	5	4	36.6	-33.7
1	5	5	26.0	26.8
1	5	6	21.2	-21.7
1	5	7	29.9	-29.1
1	5	8	10.2	9.6
1	5	9	0.0	1.4
1	6	0	19.5	-21.2
1	6	1	5.6	-3.3
1	6	2	66.7	-69.6
1	6	3	57.1	53.8
1	6	4	9.7	9.8
1	6	5	5.1	4.9
1	6	6	6.9	6.6
1	6	7	8.4	6.9
1	6	8	14.2	13.8
1	6	9	6.7	-8.0
1	6	10	5.5	5.0
1	7	0	65.8	-75.7
1	7	1	5.8	-4.8
1	7	2	6.5	3.9
1	7	3	18.9	17.7
1	7	4	44.3	-45.0
1	7	5	7.4	-4.4
1	7	6	0.0	-0.9
1	7	7	20.7	-19.8
1	7	8	3.9	3.4
1	7	9	10.7	-10.0
1	7	10	12.9	13.7
1	8	0	34.4	-36.3
1	8	1	7.5	3.9
1	8	2	20.3	-25.7
1	8	3	43.8	53.4
1	8	4	21.5	20.9
1	8	5	15.1	15.9
1	8	6	21.5	19.0
1	8	7	4.1	3.4
1	8	8	11.4	11.2
1	8	9	6.7	-5.4
1	9	0	10.6	-11.2
1	9	1	12.0	-9.1
1	9	2	13.3	13.9
1	9	3	30.0	30.5
1	9	4	19.0	-18.3
1	9	5	34.0	-33.6
1	9	6	19.3	-17.9
1	9	7	12.5	-15.3
1	9	8	7.2	6.5
1	9	9	14.1	-13.4
1	10	0	20.1	-20.9
1	10	1	7.4	-4.4
1	10	2	0.0	-2.6
1	10	3	21.4	19.4
1	10	4	3.5	4.3
1	10	5	0.0	-2.2
1	10	6	27.1	27.0
1	10	7	11.4	11.4
1	10	8	10.0	10.5
1	10	9	6.2	-5.9
1	11	0	13.4	12.3
1	11	1	38.4	38.2
1	11	2	6.3	5.0
1	11	3	16.7	-16.5
1	11	4	3.5	-5.7
1	11	5	5.3	-4.9
1	11	6	19.9	-20.5
1	11	7	15.1	-15.1
1	11	8	0.0	-0.1
1	11	9	5.1	-6.6
2	0	0	60.9	-81.1
2	0	2	27.5	-28.4
2	0	4	18.9	-23.2
2	0	6	7.6	-8.4
2	0	8	14.6	-14.6
2	0	10	0.0	3.4
2	1	0	46.7	-49.3
2	1	1	21.1	22.8
2	1	2	44.1	-39.1
2	1	3	37.4	35.5
2	1	4	10.3	11.5
2	1	5	28.3	-29.9
2	1	6	0.0	2.2
2	1	7	13.2	13.9
2	1	8	12.7	11.1
2	1	9	0.0	5.6
2	2	0	55.2	-61.0
2	2	1	0.0	5.0
2	2	2	35.6	30.6
2	2	3	14.9	14.9
2	2	4	8.6	9.5
2	2	5	33.9	-31.5
2	2	6	8.7	-8.1
2	2	7	11.1	10.4
2	2	8	0.0	-0.1
2	2	9	19.0	-18.4
2	2	10	3.7	-4.6
2	3	0	29.5	21.3
2	3	1	92.4	92.7
2	3	2	18.7	-16.7
2	3	3	25.3	-22.4
2	3	4	18.7	-17.3
2	3	5	10.0	7.9
2	3	6	20.5	18.4
2	3	7	0.0	-2.2
2	3	8	16.9	18.6
2	3	9	5.4	4.9
2	4	0	34.7	-32.1
2	4	1	111.1	117.2
2	4	2	0.0	-2.7
2	4	3	32.7	-30.0
2	4	4	11.9	10.2
2	4	5	6.0	-6.7
2	4	6	11.3	10.8
2	4	7	29.7	-28.9
2	4	8	0.0	-1.9
2	4	9	3.7	-2.8
2	4	10	13.1	-10.6
2	5	0	40.8	-44.1
2	5	1	7.5	-0.4
2	5	2	17.5	10.2
2	5	3	35.4	-32.2
2	5	4	23.1	-22.4
2	5	5	13.7	-14.2
2	5	6	45.9	45.8
2	5	7	0.0	0.1
2	5	8	12.4	14.0
2	5	9	6.2	7.1
2	5	10	6.6	4.7
2	6	0	0.0	-3.1
2	6	1	72.8	70.2
2	6	2	20.7	18.7
2	6	3	11.8	-9.3
2	6	4	3.3	2.8
2	6	5	21.4	-21.9
2	6	6	30.4	29.6
2	6	7	17.8	-15.6
2	6	8	21.4	-23.4
2	6	9	9.8	-9.9
2	7	0	21.3	-21.8
2	7	1	27.3	-28.2
2	7	2	67.7	-64.6
2	7	3	67.0	-71.8
2	7	4	13.7	12.8
2	7	5	0.0	-1.5
2	7	6	21.1	20.2
2	7	7	0.0	3.1
2	7	8	17.4	15.3
2	7	9	0.0	2.1
2	7	10	10.6	11.9
2	8	0	27.4	27.9
2	8	1	0.0	-0.0
2	8	2	14.6	-15.4
2	8	3	21.3	22.2
2	8	4	53.1	56.1
2	8	5	0.0	-2.5
2	8	6	8.1	8.1
2	8	7	27.8	-29.5
2	8	8	0.0	-0.9
2	8	9	12.5	-11.5
2	9	0	42.4	-43.9
2	9	1	12.6	-7.7
2	9	2	29.0	-27.8
2	9	3	34.9	-37.0
2	9	4	17.7	15.5
2	9	5	17.8	-15.8
2	9	6	9.0	7.7
2	9	7	5.5	-4.0
2	9	8	12.2	11.3
2	9	9	8.9	9.2
2	10	0	20.2	19.3
2	10	1	13.7	11.1
2	10	2	22.5	21.4
2	10	3	15.3	14.1
2	10	4	39.7	41.5
2	10	5	0.0	1.5
2	10	6	11.8	11.6
2	10	7	18.2	-19.9
2	10	8	0.0	-2.4
2	10	9	0.0	-2.6
2	11	0	22.2	-20.8
2	11	1	24.6	-22.4
2	11	2	9.5	-10.0
2	11	3	17.9	-19.2
2	11	4	12.5	14.6
2	11	5	24.2	-25.3
2	11	6	0.0	-0.7
2	11	7	0.0	-2.3
2	11	8	0.0	2.9
2	11	9	5.6	8.7
3	0	2	16.9	-17.8
3	0	4	52.3	42.5
3	0	6	44.2	-38.6
3	0	8	9.3	6.4
3	0	10	18.7	21.1
3	1	0	10.1	5.6
3	1	1	70.4	-58.0
3	1	2	37.4	33.3
3	1	3	51.7	52.1
3	1	4	8.9	5.8
3	1	5	13.3	13.7
3	1	6	11.2	-11.8
3	1	7	5.9	7.1
3	1	8	9.4	11.0
3	1	9	11.3	-11.5
3	2	0	42.5	-40.7
3	2	1	53.3	53.7
3	2	2	4.3	-2.0
3	2	3	29.0	-27.1
3	2	4	25.5	-22.4
3	2	5	7.2	-5.0
3	2	6	12.0	-10.3
3	2	7	14.7	-13.3
3	2	8	0.0	3.2
3	2	9	3.7	-5.6
3	2	10	12.1	12.0
3	3	0	12.4	13.6
3	3	1	4.6	5.9
3	3	2	49.4	48.8
3	3	3	0.0	-2.5
3	3	4	26.5	24.8
3	3	5	25.4	24.6
3	3	6	14.0	11.6
3	3	7	22.2	-23.5
3	3	8	8.3	8.8
3	3	9	5.2	4.5
3	3	10	5.9	-5.5
3	4	0	51.9	46.0
3	4	1	58.2	-53.7
3	4	2	15.1	-10.4
3	4	3	6.6	-5.3
3	4	4	12.5	-8.9
3	4	5	72.4	-72.3
3	4	6	20.2	-19.1
3	4	7	7.4	5.2
3	4	8	0.0	-1.3
3	4	9	10.8	11.5
3	5	0	44.7	-44.6
3	5	1	25.6	-17.6
3	5	2	67.4	70.1
3	5	3	0.0	-2.2
3	5	4	17.8	13.8
3	5	5	14.2	14.5
3	5	6	24.5	24.8
3	5	7	22.1	23.4
3	5	8	0.0	0.3
3	5	9	0.0	-5.4
3	5	10	0.0	-1.1
3	6	0	81.8	85.1
3	6	1	15.1	-10.3
3	6	2	24.6	-20.5
3	6	3	36.4	-33.6
3	6	4	8.5	8.6
3	6	5	43.9	-45.3
3	6	6	16.5	-13.8
3	6	7	0.0	-0.5
3	6	8	0.0	-3.3
3	6	9	0.0	2.2
3	7	0	29.1	-24.7
3	7	1	28.8	-25.9
3	7	2	41.2	41.2
3	7	3	38.2	-39.2
3	7	4	59.6	59.0
3	7	5	35.5	33.2
3	7	6	0.0	-3.0
3	7	7	26.0	26.9
3	7	8	9.3	7.5
3	7	9	0.0	-3.4
3	7	10	7.6	-9.4
3	8	0	34.9	32.4
3	8	1	22.4	-18.3
3	8	2	64.3	65.8
3	8	3	24.2	-22.5
3	8	4	46.3	-47.2
3	8	5	5.5	-4.5
3	8	6	0.0	-1.9
3	8	7	22.1	-20.7
3	8	8	12.5	-10.6
3	8	9	6.0	5.4
3	9	0	14.5	11.9
3	9	1	25.5	-25.9
3	9	2	0.0	3.2
3	9	3	19.4	-15.3
3	9	4	25.2	23.4
3	9	5	0.0	1.6
3	9	6	16.1	15.4
3	9	7	11.6	11.7
3	9	8	5.8	-2.9
3	9	9	8.2	7.5
3	10	0	24.6	24.4
3	10	1	45.2	-42.8
3	10	2	27.5	26.4
3	10	3	15.5	-13.1
3	10	4	13.9	-13.8
3	10	5	10.3	-8.3
3	10	6	7.8	-8.1
3	10	7	5.1	3.2
3	10	8	16.1	-14.4
3	10	9	4.5	5.6
3	11	0	8.2	-9.1
3	11	1	27.2	-24.5
3	11	2	0.0	-0.9
3	11	3	10.4	7.6
3	11	4	19.4	17.8
3	11	5	0.0	-1.9
3	11	6	6.4	4.9
3	11	7	10.7	11.0
3	11	8	11.7	-11.7
4	0	0	142.1	-142.8
4	0	2	30.6	-31.0
4	0	4	47.1	38.2
4	0	6	15.1	13.4
4	0	8	28.5	27.7
4	0	10	9.7	9.3
4	1	0	25.8	-27.3
4	1	1	0.0	2.5
4	1	2	81.7	77.9
4	1	3	3.0	-0.8
4	1	4	27.8	-23.2
4	1	5	7.5	5.2
4	1	6	7.0	5.2
4	1	7	36.7	-39.5
4	1	8	0.0	-1.0
4	1	9	10.7	-11.3
4	2	0	13.7	4.8
4	2	1	62.8	-53.8
4	2	2	40.5	-37.4
4	2	3	40.7	41.7
4	2	4	0.0	3.5
4	2	5	13.1	-12.5
4	2	6	33.4	30.3
4	2	7	0.0	0.9
4	2	8	16.4	15.7
4	2	9	3.5	5.4
4	2	10	4.4	6.0
4	3	0	39.9	39.6
4	3	1	39.2	37.9
4	3	2	23.0	15.4
4	3	3	48.1	46.2
4	3	4	24.0	22.7
4	3	5	36.7	-33.4
4	3	6	21.6	-20.7
4	3	7	14.8	-15.8
4	3	8	0.0	1.2
4	3	9	11.0	-11.0
4	3	10	6.0	-6.5
4	4	0	24.6	-19.4
4	4	1	41.3	-40.2
4	4	2	27.3	-22.1
4	4	3	4.5	-4.8
4	4	4	14.2	-14.3
4	4	5	26.5	-27.9
4	4	6	31.0	31.4
4	4	7	12.8	12.9
4	4	8	12.7	14.3
4	4	9	9.6	9.4
4	5	0	57.7	55.6
4	5	1	85.7	79.9
4	5	2	34.9	27.6
4	5	3	10.4	-10.8
4	5	4	44.8	44.0
4	5	5	9.6	-10.1
4	5	6	28.8	-27.6
4	5	7	0.0	2.2
4	5	8	10.4	-10.3
4	5	9	12.0	-11.8
4	5	10	5.0	-5.8
4	6	0	20.4	-16.9
4	6	1	36.4	-31.8
4	6	2	8.7	5.3
4	6	3	53.1	-50.8
4	6	4	38.9	-38.2
4	6	5	27.2	27.0
4	6	6	0.0	-6.3
4	6	7	0.0	2.7
4	6	8	12.0	12.9
4	6	9	6.5	6.4
4	7	0	23.1	21.5
4	7	1	14.8	13.5
4	7	2	50.5	47.5
4	7	3	27.8	26.3
4	7	4	20.5	-19.9
4	7	5	13.9	11.0
4	7	6	8.3	8.3
4	7	7	0.0	-4.1
4	7	8	11.5	-10.0
4	7	9	0.0	-3.0
4	8	0	9.4	6.4
4	8	1	29.1	-28.6
4	8	2	5.6	-5.4
4	8	3	13.2	-12.3
4	8	4	36.0	-32.8
4	8	5	21.4	20.1
4	8	6	0.0	-2.7
4	8	7	0.0	0.1
4	8	8	5.9	5.3
4	8	9	6.3	6.8
4	9	0	59.0	59.8
4	9	1	3.1	-2.0
4	9	2	0.0	-0.6
4	9	3	50.7	56.2
4	9	4	12.1	-11.1
4	9	5	16.2	-13.8
4	9	6	8.9	5.2
4	9	7	12.9	11.8
4	9	8	12.3	-11.2
4	10	0	8.9	7.6
4	10	1	0.0	1.4
4	10	2	33.5	-30.7
4	10	3	17.7	-16.3
4	10	4	0.0	-1.8
4	10	5	0.0	3.1
4	10	6	18.7	-16.7
4	10	7	18.3	16.4
4	10	8	3.5	-2.1
4	11	0	23.8	23.4
4	11	1	26.0	23.8
4	11	2	0.0	-4.1
4	11	3	0.0	-4.0
4	11	4	16.0	-13.2
4	11	5	24.3	25.6
4	11	6	9.6	-8.8
4	11	7	0.0	1.5
4	11	8	0.0	0.5
5	0	2	99.0	90.6
5	0	4	12.3	-8.6
5	0	6	60.5	64.7
5	0	8	34.4	-36.3
5	1	0	28.9	24.3
5	1	1	47.4	-44.7
5	1	2	34.7	-29.6
5	1	3	62.8	-58.1

Table 2 (*cont.*)

5	1	4	0.0	-1,0
5	1	5	19.9	-17,0
5	1	6	9.3	-9,2
5	1	7	0.0	-4,3
5	1	8	6.9	-6,6
5	1	9	4.0	4,3
5	2	0	31.0	26,1
5	2	1	56.5	-45,4
5	2	2	10.7	-8,5
5	2	3	40.2	37,4
5	2	4	53.4	52,9
5	2	5	0.0	0,7
5	2	6	26.6	24,9
5	2	7	0.0	-4,5
5	2	8	5.6	-5,1
5	2	10	9.6	-13,4
5	3	0	8.7	-5,3
5	3	1	20.5	12,4
5	3	2	25.1	-16,7
5	3	3	62.7	-41,9
5	3	4	18.1	17,0
5	3	5	27.8	-28,7
5	3	6	19.8	-17,4
5	3	7	0.0	-2,4
5	3	8	13.5	-14,6
5	3	9	12.4	11,5
5	4	0	27.8	-24,1
5	4	1	8.6	-13,3
5	4	2	0.0	-0,5
5	4	3	7.7	-3,6
5	4	4	48.4	45,5
5	4	5	46.9	44,5
5	4	6	6.0	-5,9
5	4	7	4.2	-5,2
5	4	8	6.6	7,2
5	4	9	18.3	17,1
5	5	0	43.0	-44,6
5	5	1	4.4	5,5
5	5	2	10.4	10,9
5	5	3	6.1	-5,9
5	5	4	0.0	-2,4
5	5	5	30.1	-29,2
5	5	6	0.0	-2,6
5	5	7	0.0	2,7
5	5	8	10.5	-9,5
5	5	9	6.2	7,3
5	6	0	33.2	-28,1
5	6	1	15.5	-12,6
5	6	2	49.7	45,3
5	6	3	0.0	3,5
5	6	4	11.6	13,7
5	6	5	25.2	22,0
5	6	6	0.0	-2,7
5	6	7	5.7	6,3
5	6	8	6.2	-5,4
5	6	9	0.0	1,4
5	7	0	55.4	49,7
5	7	1	7.4	7,3
5	7	2	22.6	-16,6
5	7	3	25.9	23,3
5	7	4	23.2	-20,1
5	7	5	7.1	-4,6
5	7	6	16.8	-15,9
5	7	7	10.4	-9,2
5	7	8	0.0	0,5
5	7	9	12.3	12,6
5	8	0	9.9	-8,4
5	8	1	0.0	1,9
5	8	2	26.6	-24,1
5	8	3	34.4	33,3
5	8	4	0.0	1,7
5	8	5	22.5	-21,5
5	8	6	0.0	-4,8
5	8	7	13.0	12,8
5	8	9	5.3	-4,8
5	9	0	9.6	7,2
5	9	1	38.4	33,9
5	9	2	25.2	-21,6
5	9	3	6.5	-4,2
5	9	4	8.8	-6,4
5	9	5	0.0	3,6
5	9	6	3.9	2,2
5	9	7	0.0	0,7
5	9	8	0.0	1,6
5	10	0	38.0	-35,1
5	10	1	36.2	33,3
5	10	2	20.2	-17,7
5	10	3	7.5	-5,6
5	10	4	3.9	-1,8
5	10	5	5.5	4,2
5	10	6	5.2	-5,4
5	10	7	6.5	-5,5
5	10	8	4.4	-5,0
5	11	0	18.2	-17,0
5	11	1	6.1	5,5
5	11	2	0.0	2,0
5	11	3	6.5	4,8
5	11	4	5.3	-4,0
5	11	5	9.1	8,5
5	11	6	8.5	7,1
5	11	7	5.1	5,5
5	11	8	8.2	11,4
6	0	0	117.4	108,7
6	0	2	51.8	48,5
6	0	4	3.8	3,1
6	0	6	44.2	-43,9
6	0	8	9.1	-9,8
6	1	0	35.9	31,7
6	1	1	47.8	-41,0
6	1	2	15.3	-14,9
6	1	3	18.8	-18,5
6	1	4	6.7	-6,2
6	1	5	5.8	5,6
6	1	6	7.3	-7,7
6	1	7	33.1	36,6
6	1	8	0.0	3,6
6	1	9	8.9	8,8
6	2	0	63.7	53,1
6	2	1	23.6	21,9
6	2	2	31.7	27,0
6	2	3	9.6	-6,3
6	2	4	19.7	-17,1
6	2	5	28.9	26,9
6	2	6	17.9	15,8
6	2	7	7.2	6,0
6	2	8	10.5	-8,7
6	3	0	15.9	-14,8
6	3	1	45.1	-38,6
6	3	2	31.6	-25,4
6	3	3	16.7	-14,8
6	3	4	10.4	-9,5
6	3	5	23.5	21,[illegible]
6	3	6	0.0	2,7
6	3	7	7.1	5,5
6	3	8	11.0	-12,1
6	3	9	10.4	11,5
6	4	0	16.0	13,4
6	4	1	39.2	-37,6
6	4	2	44.4	44,2
6	4	3	32.7	28,4
6	4	4	10.5	-8,6
6	4	5	0.0	-3,7
6	4	6	14.8	-15,6
6	4	7	24.5	23,4
6	4	8	13.3	-12,2
6	4	9	0.0	-2,6
6	5	0	17.7	-15,0
6	5	1	61.3	-54,2
6	5	2	18.8	18,9
6	5	3	9.3	8,0
6	5	4	26.5	-22,6
6	5	5	11.9	11,9
6	5	6	0.0	-1,2
6	5	7	16.0	17,1
6	5	8	15.4	-16,7
6	6	0	12.0	12,5
6	6	1	6.1	5,9
6	6	2	6.3	-5,7
6	6	3	7.7	7,5
6	6	4	20.2	19,3
6	6	5	24.8	24,6
6	6	6	24.6	-25,2
6	6	7	0.0	-0,4
6	6	8	0.0	-2,1
6	6	9	4.8	4,7
6	7	0	16.4	-11,2
6	7	1	21.3	-17,3
6	7	2	0.0	-0,6
6	7	3	27.5	25,8
6	7	4	0.0	-3,1
6	7	5	0.0	1,2
6	7	6	20.2	-20,7
6	7	7	0.0	-3,7
6	7	8	8.4	7,1
6	8	0	34.3	-32,0
6	8	1	45.9	45,2
6	8	2	21.8	20,6
6	8	3	6.8	-8,8
6	8	4	15.2	-15,2
6	8	5	7.1	5,6
6	8	6	0.0	3,3
6	8	7	10.5	10,3
6	9	0	15.6	-12,3
6	9	1	18.5	16,9
6	9	2	20.3	17,9
6	9	3	0.0	-1,3
6	9	4	6.9	-5,9
6	9	5	14.9	13,9
6	9	6	5.3	-4,3
6	9	7	12.3	-11,7
6	9	8	5.3	-5,9
6	10	0	19.8	-19,7
6	10	1	0.0	0,9
6	10	2	6.6	-2,2
6	10	3	0.0	-3,6
6	10	4	14.7	-13,1
6	10	5	22.8	-22,2
6	10	6	0.0	1,1
6	10	7	8.9	8,7
6	10	8	9.5	11,3
6	11	0	0.0	-1,7
6	11	1	6.4	5,0
6	11	2	23.2	20,8
6	11	3	3.8	2,9
6	11	4	0.0	2,9
6	11	5	3.6	4,5
6	11	6	7.2	8,0
6	11	7	0.0	3,7
7	0	2	0.0	4,1
7	0	4	58.9	-54,9
7	0	6	29.2	-31,0
7	0	8	0.0	0,7
7	1	0	14.0	-11,6
7	1	1	61.7	58,7
7	1	2	11.7	9,1
7	1	3	3.8	4,5
7	1	4	35.8	-37,0
7	1	5	27.4	27,2
7	1	6	12.7	11,9
7	1	7	0.0	1,3
7	1	8	0.0	2,5
7	2	0	26.4	23,4
7	2	1	18.5	-14,8
7	2	2	32.9	-29,6
7	2	3	3.9	-2,9
7	2	4	34.1	-33,0
7	2	5	18.8	18,2
7	2	6	6.0	-2,6
7	2	7	5.6	-5,7
7	3	0	5.1	0,5
7	3	1	5.1	-6,5
7	3	2	34.5	-26,9
7	3	3	66.5	62,2
7	3	4	18.8	-18,9
7	3	5	0.0	-3,9
7	3	6	0.0	-0,4
7	3	7	10.3	9,8
7	3	8	5.7	5,1
7	3	9	3.9	-5,0
7	4	0	6.0	-2,6
7	4	1	48.0	41,2
7	4	2	38.8	-34,5
7	4	3	6.9	5,9
7	4	4	21.3	-21,2
7	4	5	0.0	5,7
7	4	6	10.2	8,7
7	4	7	9.4	10,0
7	4	8	5.5	7,0
7	4	9	11.8	-15,1
7	5	0	41.2	35,9
7	5	1	20.9	18,6
7	5	2	59.6	-53,4
7	5	3	0.0	-4,1
7	5	4	15.7	15,5
7	5	5	21.2	21,8
7	5	6	9.2	-8,1
7	5	7	10.5	-10,5
7	5	8	3.7	5,2
7	6	0	13.1	-8,3
7	6	1	19.1	15,7
7	6	2	15.8	-11,7
7	6	3	14.1	12,7
7	6	4	0.0	4,8
7	6	5	16.2	18,6
7	6	6	8.0	-8,8
7	6	7	0.0	-4,8
7	6	8	6.0	7,5
7	7	0	11.5	-9,2
7	7	1	0.0	3,4
7	7	2	6.9	-8,1
7	7	3	0.0	2,0
7	7	4	46.0	-45,5
7	7	5	0.0	-2,3
7	7	6	0.0	2,2
7	7	7	13.6	-14,2
7	7	8	0.0	4,5
7	8	0	20.1	-15,2
7	8	1	12.4	-9,0
7	8	2	30.1	-28,8
7	8	3	17.3	14,9
7	8	4	15.3	13,9
7	8	5	13.8	12,6
7	8	6	26.1	27,1
7	8	7	0.0	2,3
7	9	0	11.0	-11,3
7	9	1	15.7	-14,3
7	9	2	0.0	1,3
7	9	3	17.9	15,9
7	9	4	0.0	0,3
7	9	5	15.3	-15,5
7	9	6	17.3	-17,5
7	9	7	10.6	-11,5
7	10	0	11.6	-10,7
7	10	1	3.9	-3,8
7	10	2	0.0	-2,4
7	10	3	11.7	10,9
7	10	4	0.0	5,2
7	10	5	8.1	7,6
7	10	6	17.8	19,6
7	10	7	0.0	4,5
7	11	0	11.4	11,3
7	11	1	15.2	11,7
7	11	2	7.6	6,6
7	11	3	13.0	-11,9
7	11	4	3.0	5,6
7	11	5	3.3	-5,6
7	11	6	9.3	-10,9
7	11	7	10.3	-16,1
8	0	0	76.4	-69,9
8	0	2	55.1	49,0
8	0	4	37.9	-34,7
8	0	6	0.0	2,2
8	0	8	0.0	-1,0
8	1	0	48.3	42,9
8	1	1	31.5	28,9
8	1	2	25.8	-25,8
8	1	3	14.3	13,9
8	1	4	8.4	-6,2
8	1	5	0.0	-2,0
8	1	6	8.1	9,6
8	1	7	0.0	0,0
8	1	8	7.2	6,0
8	2	0	44.6	-41,4
8	2	1	0.0	5,4
8	2	2	28.1	-23,7
8	2	3	12.5	11,4
8	2	4	17.0	17,0
8	2	5	13.4	-12,5
8	2	6	7.0	-7,4
8	2	7	3.6	-3,9
8	3	0	0.0	0,7
8	3	1	29.4	26,5
8	3	2	7.0	5,5
8	3	3	11.1	9,4
8	3	4	10.4	-9,5
8	3	5	12.7	-12,4
8	3	6	15.1	15,0
8	3	7	7.1	-5,8
8	3	8	10.8	13,2
8	4	0	7.9	-6,3
8	4	1	71.0	65,3
8	4	2	38.4	-31,9
8	4	3	39.3	-36,1
8	4	4	17.1	16,9
8	4	5	0.0	-5,4
8	4	6	0.0	3,8
8	4	7	14.7	-15,4
8	5	0	44.4	-41,0
8	5	1	33.8	-29,6
8	5	2	0.0	-1,4
8	5	3	0.0	2,5
8	5	4	0.0	2,1
8	5	5	0.0	0,1
8	5	6	13.4	13,4
8	5	7	0.0	-5,1
8	5	8	15.2	18,4
8	6	0	5.7	-3,9
8	6	1	26.6	22,1
8	6	2	21.4	17,8
8	6	3	20.9	18,9
8	6	4	8.4	7,5
8	6	5	26.5	-26,1
8	6	6	14.0	14,0
8	6	7	16.8	-15,7
8	6	8	6.1	-8,1
8	7	0	10.0	-7,1
8	7	1	15.3	-13,4
8	7	2	23.7	-17,8
8	7	3	34.2	-31,8
8	7	4	0.0	4,2
8	7	5	13.6	-14,1
8	7	6	10.0	10,0
8	7	7	10.8	10,6
8	7	8	12.0	15,1
8	8	0	22.3	21,1
8	8	1	9.1	-7,4
8	8	2	10.0	-8,8
8	8	3	32.3	30,5
8	8	4	32.5	33,1
8	8	5	11.9	-9,2
8	8	6	0.0	0,0
8	8	7	9.3	-9,8
8	9	0	37.9	-35,3
8	9	1	13.9	12,8
8	9	2	10.6	-10,4
8	9	3	37.5	-38,1
8	9	4	0.0	1,0
8	9	5	10.0	-8,7
8	9	6	0.0	3,9
8	9	7	4.9	-4,6
8	10	0	0.0	2,3
8	10	1	11.1	10,1
8	10	2	21.6	21,3
8	10	3	0.0	-0,4
8	10	4	15.9	14,9
8	10	5	9.8	9,7
8	10	6	6.9	9,5
8	10	7	10.5	-15,8
8	11	0	16.5	-18,6
8	11	1	19.7	-22,1
8	11	2	9.8	-9,7
8	11	3	7.1	-7,3
8	11	4	0.0	-1,5
8	11	5	12.6	-14,7
8	11	6	4.1	6,1
9	0	2	14.5	-13,7
9	0	4	17.6	18,2
9	0	6	21.2	-23,4
9	0	8	14.0	14,8
9	1	0	0.0	0,9
9	1	1	37.3	-34,0
9	1	2	7.3	5,7
9	1	3	20.3	19,7
9	1	4	6.0	5,[illegible]
9	1	5	4.1	-3,4
9	1	6	0.0	1,2
9	1	7	0.0	-0,1
9	1	8	7.2	8,8
9	2	0	33.1	-34,2
9	2	1	19.1	16,1
9	2	2	16.9	14,0
9	2	3	13.5	-12,2
9	2	4	0.0	-3,3
9	2	5	5.7	-6,6
9	2	6	0.0	-1,1
9	2	7	6.6	-6,5
9	3	0	28.9	-26,7
9	3	1	20.5	19,3
9	3	2	50.9	50,2
9	3	3	0.0	-1,1
9	3	4	4.2	-3,4
9	3	5	9.9	9,9
9	3	6	15.6	15,6
9	4	0	14.6	12,1
9	4	1	8.4	-7,2
9	4	2	15.9	17,0
9	4	3	17.8	-12,0
9	4	4	13.2	-14,3
9	4	5	36.1	-39,1
9	4	6	8.0	8,5
9	4	7	0.0	-2,6
9	5	0	0.0	-1,4
9	5	1	5.9	-2,1
9	5	2	40.6	39,5
9	5	3	15.8	-15,8
9	5	4	18.5	19,3
9	5	5	6.7	6,5
9	5	6	10.9	12,3
9	5	7	10.2	13,2
9	6	0	52.8	54,9
9	6	1	0.0	-3,3
9	6	2	5.9	-4,5
9	6	3	22.1	-22,2
9	6	4	12.1	-12,5
9	6	5	21.5	-21,0
9	6	6	12.7	-12,1
9	6	7	5.4	-5,8
9	7	0	18.1	16,8
9	7	1	9.3	-8,0
9	7	2	16.8	-14,5
9	7	3	25.7	-24,4
9	7	4	41.3	39,7
9	7	5	8.8	8,7
9	7	6	11.3	9,9
9	7	7	14.8	18,4
9	8	0	17.8	18,1
9	8	1	0.0	-2,6
9	8	2	27.6	26,7
9	8	3	32.0	-32,6
9	8	4	9.1	-8,3
9	8	5	0.0	3,8
9	8	6	10.4	-10,7
9	8	7	8.6	-10,5
9	9	0	5.6	3,7
9	9	1	7.9	-7,8
9	9	2	0.0	1,1
9	9	3	7.5	-6,1
9	9	4	14.9	10,8
9	9	5	17.6	16,6
9	9	6	10.7	11,5
9	10	0	17.2	17,8
9	10	1	15.1	-14,0
9	10	2	15.1	13,9
9	10	3	9.3	-5,8
9	10	4	0.0	-5,1
9	10	5	11.9	-11,7
9	10	6	5.7	-7,2
9	11	0	6.2	-6,3
9	11	1	25.5	-27,8
9	11	2	0.0	-0,3
9	11	3	8.5	9,9
9	11	4	3.5	5,6
10	0	0	19.2	18,1
10	0	2	42.4	-41,3
10	0	4	23.7	23,8
10	0	6	13.8	16,5
10	1	0	15.9	-14,1
10	1	1	8.5	7,6
10	1	2	12.7	13,1
10	1	3	17.5	-16,4
10	1	4	0.0	0,2
10	1	5	11.2	12,9
10	1	6	0.0	0,5
10	1	7	19.7	-26,0
10	2	0	6.0	-4,2
10	2	1	32.3	-29,4
10	2	2	18.1	-18,0
10	2	3	11.1	10,1
10	2	4	8.0	7,9
10	2	5	0.0	-0,4
10	2	6	13.6	13,4
10	3	0	9.5	7,2
10	3	1	8.5	-8,0
10	3	2	14.7	12,6
10	3	3	21.7	23,0
10	3	4	16.9	17,4
10	3	5	17.8	-19,0
10	3	6	14.4	-14,8
10	4	0	12.8	-11,5
10	4	1	35.4	-34,2
10	4	2	12.6	-11,2
10	4	3	0.0	-0,9
10	4	4	7.8	-6,6
10	4	5	0.0	-2,5
10	4	6	7.4	7,4
10	4	7	8.3	8,7
10	5	0	22.0	20,9
10	5	1	20.4	19,4
10	5	2	13.1	15,0
10	5	3	11.4	12,6
10	5	4	24.2	25,7
10	5	5	0.0	-1,2
10	5	6	17.1	-18,8
10	5	7	6.4	-6,0
10	6	0	0.0	-4,7
10	6	1	26.9	-27,4
10	6	2	8.1	9,0
10	6	3	6.8	-7,9
10	6	4	15.6	-15,8
10	7	0	12.2	11,8
10	7	1	20.0	18,8
10	7	2	32.4	34,1
10	7	3	11.3	11,5
10	7	4	15.2	-15,2
10	7	5	7.5	7,5
10	8	0	0.0	1,6
10	8	1	20.1	18,7
10	8	2	13.1	-13,2
10	8	3	14.4	-10,8
10	8	4	20.8	-19,4
10	8	5	10.3	-8,7
10	9	0	22.1	20,6
10	9	1	5.2	6,2
10	9	2	5.0	4,5
10	9	3	19.8	21,0
10	9	4	0.0	2,0
10	10	0	4.9	4,2
10	10	1	5.9	-4,1
10	10	2	15.4	-16,2
10	10	3	11.3	-9,6
10	10	4	9.3	-10,1
10	10	5	5.0	3,8
10	11	0	12.8	13,5
10	11	1	9.4	11,4
10	11	2	6.3	-7,7
10	11	3	0.0	[illegible]
10	11	4	3.9	5,7
11	0	2	19.8	21,7
11	0	4	9.5	9,2
11	0	6	28.1	34,4
11	1	0	7.2	6,4
11	1	1	16.5	-18,2
11	1	2	9.0	-9,4
11	1	3	17.7	-10,7
11	1	4	7.2	7,1
11	1	5	19.2	-21,1
11	1	6	5.3	-5,6
11	2	0	0.0	0,2
11	2	1	8.2	-7,7
11	2	2	8.0	7,6
11	2	3	14.5	13,0
11	2	4	16.8	19,8
11	2	5	0.0	4,0
11	2	6	5.2	5,5
11	3	0	0.0	-1,9
11	3	1	16.4	16,1
11	3	2	0.0	-1,9
11	3	3	24.4	-26,1
11	3	5	7.5	-7,7
11	3	6	5.7	-7,6
11	4	0	4.0	-4,3
11	4	1	0.0	-1,1
11	4	2	6.8	8,1
11	4	3	11.2	-11,2
11	4	4	14.5	16,0
11	4	5	27.5	31,0
11	5	0	5.6	-6,3
11	5	1	5.5	-5,0
11	5	2	0.0	-5,4
11	5	3	0.0	1,1
11	5	4	16.1	-15,6
11	5	5	9.0	-11,7
11	5	6	4.7	-7,0
11	6	0	27.0	-30,2
11	6	1	9.3	-10,3
11	6	2	12.8	-12,6
11	6	3	14.7	15,0
11	6	4	0.0	-1,4
11	7	0	22.0	22,5
11	7	1	0.0	0,9
11	7	2	12.2	-12,1
11	7	3	12.0	11,9
11	7	5	11.9	-13,2
11	8	0	10.5	-10,5
11	8	1	0.0	2,8
11	8	2	9.9	-10,3
11	8	3	15.6	15,6
11	8	4	12.0	12,1
11	9	0	3.2	4,5
11	9	1	18.9	18,5
11	9	2	0.0	1,8
11	9	3	9.5	9,4
11	9	4	11.1	-13,0
11	10	0	9.6	-9,2
11	10	1	22.7	23,8
11	10	2	9.4	-10,9
11	10	3	8.2	-9,5
11	11	0	7.8	-10,6
11	11	3	3.2	3,8
12	0	0	51.8	54,2
12	0	4	14.5	17,4
12	1	0	0.0	-0,6
12	1	1	11.2	-10,7
12	1	2	7.1	-8,0
12	1	3	12.3	-13,2
12	1	4	8.1	9,2
12	2	0	18.5	17,4
12	2	1	10.5	10,3
12	2	2	21.6	22,7
12	2	3	12.1	-12,7
12	2	4	13.3	-16,1
12	2	5	12.5	18,5
12	3	0	0.0	0,8
12	3	1	10.3	-10,2
12	3	2	15.8	-16,7
12	3	3	15.8	-14,3
12	3	5	13.7	19,5
12	4	0	0.0	4,7
12	4	1	7.9	-8,0
12	4	2	17.9	20,4
12	4	3	18.4	19,1
12	4	4	9.9	-10,1
12	4	5	5.3	6,7
12	5	1	17.8	-20,3
12	5	2	11.3	-12,1
12	5	3	8.1	8,5
12	5	4	13.1	-15,9
12	6	0	8.8	9,0
12	6	1	12.0	11,1
12	6	2	5.3	-6,9
12	6	4	13.4	17,8
12	7	0	8.6	-7,4
12	7	1	9.9	-9,6
12	7	2	11.1	-11,3
12	8	0	10.6	-12,2
12	8	1	13.7	14,2
12	8	3	5.3	-5,1
12	9	0	4.4	-6,0
12	9	2	7.7	8,8
12	10	1	7.0	-8,9
13	1	0	6.7	-6,0
13	1	1	13.0	16,5
13	1	2	13.1	16,4
13	1	3	9.7	13,7
13	2	0	8.5	8,3
13	2	2	8.4	-8,2
13	3	0	11.7	12,0
13	3	1	10.8	-11,7
13	3	2	9.4	-10,9
13	3	3	19.6	28,3
13	4	0	3.5	3,4
13	4	1	10.3	12,4
13	4	2	19.3	-21,9
13	4	3	6.4	6,5
13	5	1	5.6	9,1
13	5	2	15.6	-21,8
13	6	0	9.8	-11,4
13	6	1	5.9	7,6
13	7	0	13.6	-17,2
13	7	2	10.2	15,0
14	0	0	32.6	-45,4
14	1	0	8.1	-7,0
14	1	1	7.0	9,5
14	2	0	7.8	-10,7
14	3	0	6.4	7,2

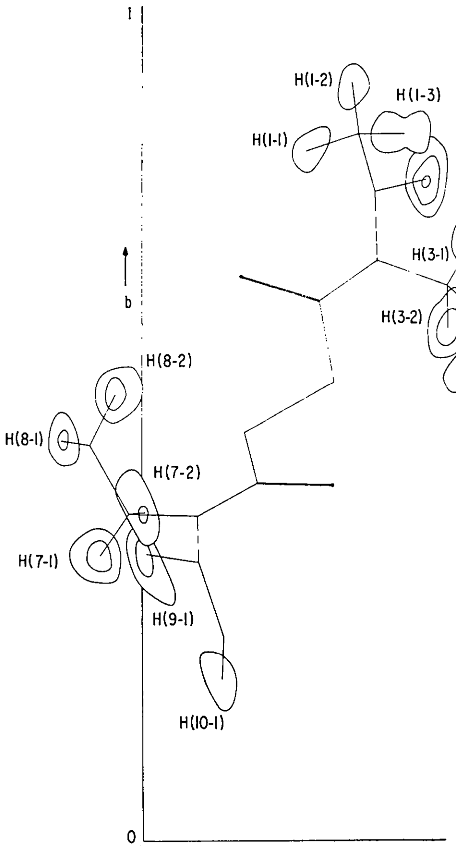


Fig. 1. A projection along the c axis of sections of a difference map for the location of hydrogen atoms. Contours are at intervals of 0·25 e.Å^{-3}, starting with the 0·25 e.Å^{-3} contour.

e.g. Karle & Karle, 1963, 1964, 1965*a*,*b*; Karle, Britts & Gum, 1964; Karle & Britts, 1966). The phase determination for this crystal was routine. Two letters a and b representing unknown signs were specified as needed in the course of the phase determination using the Σ_2 formula. These assignments and the three origin specifying signs are shown in Table 1. The Σ_2 formula (Hauptman & Karle, 1953) is the probability analog of the third general inequality of Karle & Hauptman [1950, equation (34)]. In applying the Σ_2 formula only the largest $|E|$ values were employed in the initial stages so that $P_+(E_{\mathbf{h}})$ (Hauptman & Karle, 1953; Woolfson, 1954) was always greater than 0·98.

During the course of the phase determination, it became apparent that both a and b had to be positive. The signs obtained were used to compute an E map. A three-dimensional E map computed with ~10 terms per atom in the asymmetric unit usually reveals the structure for an equal atom problem. In the present case, with four S atoms and twelve C and N atoms, the initial E map with 241 terms revealed the structure but there were several spurious peaks as large as some of the peaks for the C atoms. The addition of more data suppressed the spurious peaks.

The coordinates of the sixteen atoms as obtained from the E map were refined by means of a least-squares adjustment using a modification of the ORFLS program (Busing, Martin & Levy, 1962). The function which was minimized was $\Sigma(F_o-F_c)^2$. The refinement was initially carried out with the data from the b axis alone. Individual scale factors for each layer were varied during the isotropic refinement. Since the exposures were controlled and since the data had been

Table 3. *Fractional coordinates* for tetraethylthiuram disulfide*

Thermal parameters are of the form $T=\exp\left[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)\right]$. Each thermal parameter is multiplied by 10^4.

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
S(1)	0·6688	0·6721	0·7722	34	32	221	8	−37	7
S(2)	0·8293	0·5470	0·9482	47	19	116	−7	−28	5
S(3)	0·6739	0·4852	0·9138	52	23	101	−12	6	−11
S(4)	0·8267	0·4220	0·6569	41	52	182	2	24	−33
C(1)	0·8693	0·8464	0·8921	66	35	170	0	−7	−8
C(2)	0·8988	0·7772	0·7742	71	17	127	−6	2	11
C(3)	1·0227	0·6632	0·8991	32	36	131	8	−19	−10
C(4)	1·0882	0·6192	0·7696	50	61	146	22	−1	−13
C(5)	0·8036	0·6456	0·8470	39	24	104	7	−10	−18
C(6)	0·6961	0·4269	0·7366	39	23	129	1	−2	−13
C(7)	0·4769	0·3973	0·7585	38	28	159	−1	−2	−10
C(8)	0·4101	0·4715	0·6864	56	39	193	22	−5	−1
C(9)	0·5954	0·3331	0·5475	77	30	162	7	−24	−45
C(10)	0·6367	0·2442	0·5863	85	49	289	0	−8	−57
N(1)	0·9019	0·6936	0·8419	36	21	98	0	−14	−1
N(2)	0·5947	0·3852	0·6870	36	30	135	2	−17	−9
Standard deviations									
S	0·0002	0·0002	0·0003	3	3	5	1	2	2
C	0·0009	0·0009	0·0013	10	15	30	5	8	7
N	0·0007	0·0007	0·0010	8	10	20	3	5	5

* Coordinates are so chosen that they may be substituted directly into the equations representing the least-squares planes.

placed on an absolute scale by means of a K curve, the individual scale factors for each layer were near unity. During the anisotropic refinement the scale factors, as obtained from the isotropic refinement, were kept constant.

An independent refinement was performed with data where the intensities from both the a and b axes were cross-correlated; hence a single scale factor was needed for all the data. The results from both refinements were well within the limits of the standard deviations.

The final R value was 9·4% for the observed data. The observed and calculated structure factors are listed in Table 2. A difference electron density map (Fig. 1) revealed the positions of sixteen of the twenty hydrogen atoms. The C–H bond lengths as determined from the difference map ranged from 0·92 to 1·28 Å.

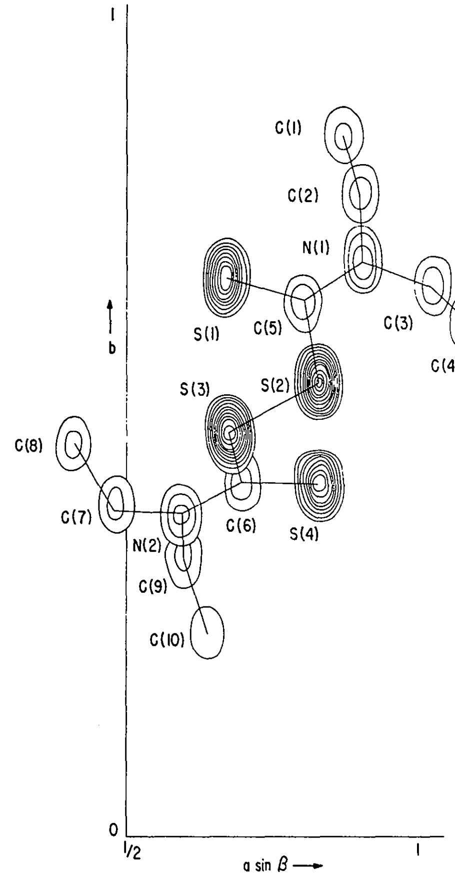


Fig. 2. A projection along the c axis of sections of the final electron density map for tetraethylthiuram disulfide. Contours are at intervals of 2·5 e.Å^{-3}, starting with the 2·5 e.Å^{-3} contour.

The parameters for the heavy atoms are given in Table 3 and the hydrogen coordinates as read from the difference map are shown in Table 4. Sections from an electron density map showing the heavy atoms are illustrated in Fig. 2. They are projected along [001]. The bond distances and angles are shown in Fig. 3.

The structure

The structural feature of particular interest for tetraethylthiuram disulfide is the conformation of the mole-

Table 4. *The approximate coordinates for the hydrogen atoms as determined from the difference electron density map*

	Bonded to	x	y	z
H(1–1)	C(1)	0·783	0·823	0·950
H(1–2)	C(1)	0·860	0·907	0·852
H(1–3)	C(1)	0·950	0·845	0·967
H(2–1)	C(2)	0·988	0·790	0·747
H(3–1)	C(3)	1·067	0·717	0·930
H(3–2)	C(3)	1·023	0·610	0·990
H(4–1)	C(4)	1·050	0·665	0·665
H(4–2)	C(4)	1·148	0·592	0·827
H(4–3)	C(4)	1·057	0·560	0·725
H(7–1)	C(7)	0·428	0·338	0·720
H(7–2)	C(7)	0·505	0·390	0·872
H(8–1)	C(8)	0·363	0·478	0·713
H(8–2)	C(8)	0·455	0·533	0·697
H(9–1)	C(9)	0·505	0·342	0·500
H(10–1)	C(10)	0·635	0·190	0·498

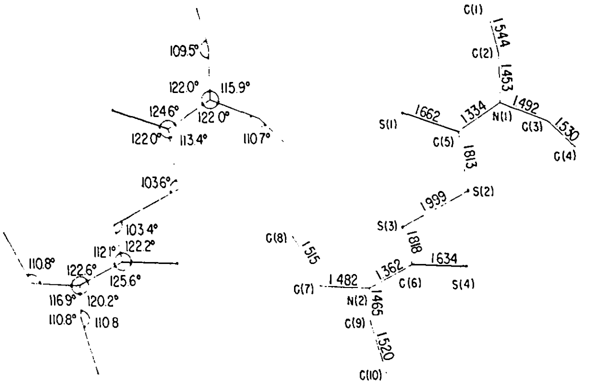


Fig. 3. Bond distances and angles. The standard deviations for the bond lengths range from 0·005 Å for the S–S bond to 0·025 Å for the C–C bonds, and the standard deviations for the angles range from 0·3° for those angles including sulfur to 1·0° for those angles where sulfur is not included.

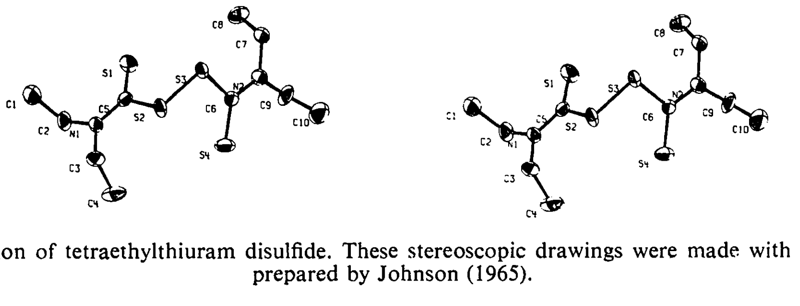


Fig. 4. Stereoconfiguration of tetraethylthiuram disulfide. These stereoscopic drawings were made with a computing program prepared by Johnson (1965).

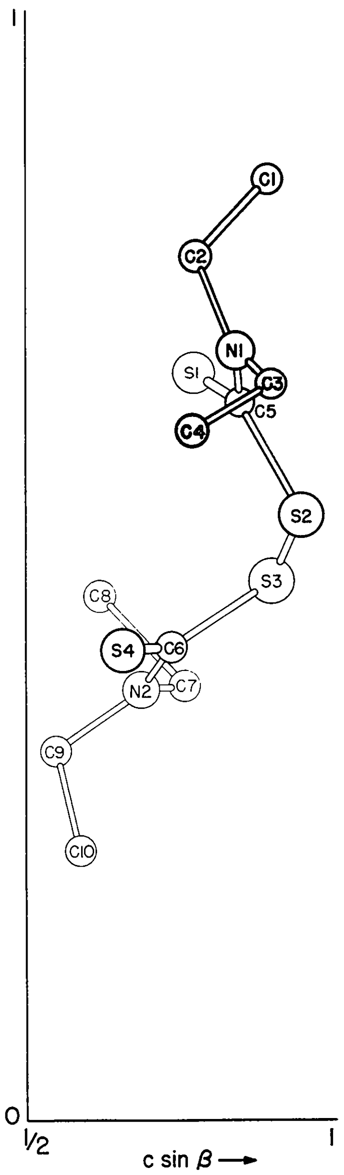
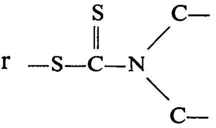
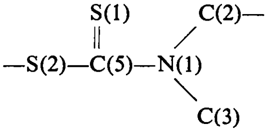
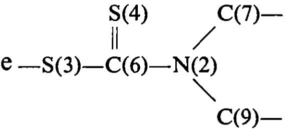


Fig. 5. Configuration of tetraethylthiuram disulfide viewed along the *a* axis.

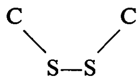
cule. Except for the terminal methyl groups, the molecule consists of two planar  $-\mathrm{S}-\overset{\overset{\displaystyle\mathrm{S}}{\|}}{\mathrm{C}}-\mathrm{N}{<}^{\mathrm{C}-}_{\mathrm{C}-}$ groups, which are nearly perpendicular to each other. Figs. 4 and 5 illustrate this feature. The four terminal methyl groups are not included in these planes. The equations for the least-squares planes are, for the

 $-\mathrm{S(2)}-\overset{\overset{\displaystyle\mathrm{S(1)}}{\|}}{\mathrm{C(5)}}-\mathrm{N(1)}{<}^{\mathrm{C(2)}-}_{\mathrm{C(3)}}$ group:

$$-2{\cdot}6425x+6{\cdot}6226y+7{\cdot}6874z=8{\cdot}6685\,, \qquad (1)$$

and for the  $-\mathrm{S(3)}-\overset{\overset{\displaystyle\mathrm{S(4)}}{\|}}{\mathrm{C(6)}}-\mathrm{N(2)}{<}^{\mathrm{C(7)}-}_{\mathrm{C(9)}-}$ group:

$$2{\cdot}3510x-0{\cdot}1270y+4{\cdot}7892z=-0{\cdot}2372\,. \qquad (2)$$

The dihedral angle between these planes, which is in effect the dihedral angle in the  $\overset{\mathrm{C}\quad\mathrm{C}}{\diagdown\ \diagup}\atop{\mathrm{S}-\mathrm{S}}$ group, is 96°25′. Deviations of the individual atoms from the planes are listed in Table 5. The deviations show that the six atoms in each group are not completely coplanar but that there could be small rotations about the C(5)–N(1) and C(6)–N(2) bonds of the order of 4°. It is interesting to note that the three bonds to each N atom are coplanar rather than in a pyramidal arrangement.

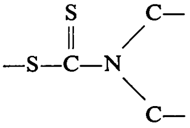
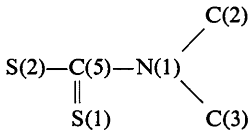
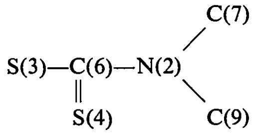
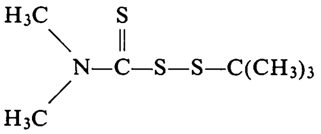
The  $-\mathrm{S}-\overset{\overset{\displaystyle\mathrm{S}}{\|}}{\mathrm{C}}-\mathrm{N}{<}^{\mathrm{C}-}_{\mathrm{C}-}$ groups in the present study can be compared with similar groups contained in:

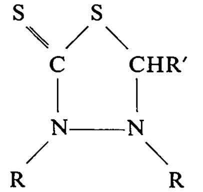
Table 5. *Distances of atoms from least-squares planes*

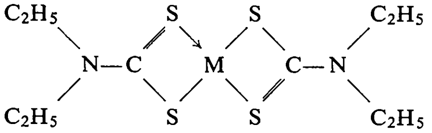
 $\mathrm{S(2)}-\underset{\underset{\displaystyle\mathrm{S(1)}}{\|}}{\mathrm{C(5)}}-\mathrm{N(1)}{<}^{\mathrm{C(2)}}_{\mathrm{C(3)}}$ group,

 $\mathrm{S(3)}-\underset{\underset{\displaystyle\mathrm{S(4)}}{\|}}{\mathrm{C(6)}}-\mathrm{N(2)}{<}^{\mathrm{C(7)}}_{\mathrm{C(9)}}$ group,

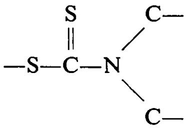
Equation (1)		Equation (2)	
	Δ		Δ
N(1)	0·014 Å	N(2)	0·036 Å
C(5)	−0·005	C(6)	−0·018
S(1)	−0·049	S(4)	−0·031
S(2)	0·052	S(3)	0·037
C(2)	0·055	C(7)	−0·053
C(3)	−0·067	C(9)	0·030

(*A*)  (Mitchell, 1966)

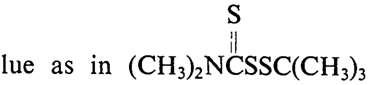
(*B*)  (Karle & Karle, 1965)

(*C*) 

where M = Cu, Ni, Zn. (Bonamico, Dessy, Mariani, Vaciago & Zambonelli, 1965; Bonamico, Dessy, Mugnoli, Vaciago & Zambonelli, 1965; Bonamico, Mazzone, Vaciago & Zambonelli, 1965).

In each case the  group is essentially planar and the C–N bond adjacent to the S atoms is quite short, 1·31–1·36 Å, while the other C–N bonds are in the range 1·44–1·49 Å.

The two C = S bonds in tetraethylthiuram disulfide average 1·65 Å. These values are nearly the same as those found for C = S in compound (*A*), 1·66 Å, compound (*B*), 1·65 Å, and allylthiourea, 1·66 Å (Dragonette & Karle, 1965).

The configuration about the S–S bond is similar to that found in hydrogen peroxide (Abrahams, Collin & Lipscomb, 1951). The dihedral angle formed by the planes containing the S–S or O–O bond and an adjacent atom is 96·4° for the tetraethylthiuram disulfide and 93·6° for the hydrogen peroxide. In *N,N'*-diglycyl-L-cystine dihydrate (Yakel & Hughes, 1954) and in L-cystine hydrochloride (Steinrauf, Peterson & Jensen, 1958) the dihedral angle in the CSSC group is somewhat larger, 101°. The S–S bond in the L-cystine derivatives was reported to be 2·04 Å while the S–S bond in  $(C_2H_5)_2N\overset{S}{\overset{\|}{C}}S\,S\overset{S}{\overset{\|}{C}}N(C_2H_5)_2$ was found to be 2·00 Å, the same value as in  $(CH_3)_2N\overset{S}{\overset{\|}{C}}SSC(CH_3)_3$ (Mitchell, 1966).

We are indebted to Mr S. Brenner for preparing the various computer programs and to Dr D. Mitchell for executing the computations.

References

Abrahams, S. C., Collin, R. L. & Lipscomb, W. N. (1951). *Acta Cryst.* **4**, 15.

Bonamico, M., Dessy, G., Mariani, C., Vaciago, A. & Zambonelli, L. (1965). *Acta Cryst.* **19**, 619.

Bonamico, M., Dessy, G., Mugnoli, A., Vaciago, A. & Zambonelli, L. (1965). *Acta Cryst.* **19**, 886.

Bonamico, M., Mazzone, G., Vaciago, A. & Zambonelli, L. (1965). *Acta Cryst.* **19**, 898.

Busing, W. R., Martin, K. O. & Levy, H. A. (1962). *ORFLS.* Oak Ridge National Laboratory, Oak Ridge, Tennessee, U.S.A.

Dragonette, K. S. & Karle, I. L. (1965). *Acta Cryst.* **19**, 978.

Grabar, D. G. & McCrone, W. C. (1950). *Anal. Chem.* **22**, 620.

Hauptman, H. & Karle, J. (1953). *Solution of the Phase Problem I. The Centrosymmetric Crystal.* A.C.A. Monograph No. 3. Pittsburgh: Polycrystal Book Service.

Johnson, C. K. (1965). *ORTEP ORNL*-3794. Oak Ridge National Laboratory, Oak Ridge, Tennessee, U.S.A.

Karle, I. L. & Britts, K. (1966). *Acta Cryst.* **20**, 118.

Karle, I. L., Britts, K. & Gum, P. (1964). *Acta Cryst.* **17**, 496.

Karle, I. L. & Karle, J. (1963). *Acta Cryst.* **16**, 969.

Karle, I. L. & Karle, J. (1964). *Acta Cryst.* **17**, 1356.

Karle, I. L. & Karle, J. (1965*a*). *Acta Cryst.* **18**, 345.

Karle, I. L. & Karle, J. (1965*b*). *Acta Cryst.* **19**, 92.

Karle, J. & Hauptman, H. (1950). *Acta Cryst.* **3**, 181.

Mitchell, D. (1966). Abstracts A.C.A. Austin, Texas.

Steinrauf, L. K., Peterson, J. & Jensen, L. H. (1958). *J. Amer. Chem. Soc.* **80**, 3835.

Woolfson, M. M. (1954). *Acta Cryst.* **7**, 61.

Yakel, H. L. & Hughes, E. W. (1954). *Acta Cryst.* **7**, 291.