ACTA CHEMICA SCANDINAVICA 22 (1968) 2851–2866

Crystal Structures of Tetrabromoethylene and of 1:1 Pyrazine Adducts of Tetrabromo- resp. Tetraiodoethylene

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Details are presented of three-dimensional crystal structure analyses of tetrabromoethylene, of its 1:1 pyrazine adduct and of the corresponding tetraiodoethylene-pyrazine compound. The packing of the acceptor molecules is left virtually unaltered after the introduction of the less voluminous pyrazine molecules into the lattice of the tetrahalogenoethylenes. Infinite chains of alternating donor and acceptor molecules, depending on nitrogen-halogen bonds, are present in both adducts which are, however, not isomorphous. The N···Hal bond length is 0.04 Å shorter in the case of iodine (2.979) than in the case of bromine (3.018).

We expected that solid 1:1 addition compounds might be formed by pyrazine and tetrabromo- resp. tetraiodoethylene with crystal structures exihibiting infinite chains of alternating donor and acceptor molecules based on nitrogen-halogen charge-transfer bonds. In these chains halogen atoms were expected to be situated near the plane of the pyrazine ring to which they are directly linked, with a nearly linear arrangement: carbon-halogen-nitrogen. As the acceptor molecule is somewhat larger than the donor molecule and the bromine, resp. iodine atoms will play a dominating role in its van der Waals interactions, we further suspected the mutual arrangements of these molecules to be rather similar in acceptor and in adduct crystals. The correctness of these expectations have been confirmed,[1,2] here we present details of the three crystal structure determinations.

EXPERIMENTAL

The two addition compounds were prepared by evaporation of the solvent (at about 5°C) from solutions in ethyl ether containing the donor and acceptor components in the molar ratio 1:1. Monoclinic plates, particularly thin in the case of the tetraiodoethylene adduct, and developed parallel to the (100) plane, were obtained, and turned out to be suitable for X-ray investigation. Crystal structure determinations of these compounds and of tetrabromoethylene were carried out using three-dimensional diffraction material. For tetraiodoethylene available data [3] were considered sufficiently accurate for our purpose of comparison.

Table 1. Lattice parameters. (Estimated standard deviations in parantheses).

	Tetrabromoethylene	Tetrabromoethylene-pyrazine	Tetraiodoethylene-pyrazine
a (Å)	14.181 (.001)	11.803 (.002)	12.371 (.003)
b (Å)	4.136 (.001)	4.161 (.005)	4.472 (.006)
c (Å)	12.154 (.001)	12.094 (.004)	12.676 (.007)
β (°)	111.99 (.01)	113.08 (.02)	117.57 (.03)

Crystals of the two addition compounds are not stable in the air and precise measurements of their lattice constants were carried out using Weissenberg technique with barium fluoride as a calibration substance. In the case of tetrabromoethylene Guinier technique was employed. Lattice parameters thus arrived at are presented in Table 1. For all three crystal species the space group is $P2_1/c$ and the unit cells all contain *four* molecules.

The three-dimensional intensity material was collected from photometric measurements of integrated Weissenberg films taken with filtered MoK radiation. The intensity of the weakest reflexions was estimated visually. In the case of tetrabromoethylene the crystals were very small and of nearly cylindrical shape, and calculations showed that absorption corrections were not essential. For the addition compounds, however, such corrections turned out to be important and they were carried out using the numerical method of Busing and Levy.[4] Weissenberg diagrams were taken with rotation about the monoclinic b axes. Further, results derived for the two addition compounds from precession cross-layer diagrams with rotation about [100] and [101] were included in the calculations. In the case of tetrabromoethylene the material was supplemented by diffractometer data about [100] and [010].

STRUCTURE DETERMINATIONS

The heavy atom procedure was used starting with the computation of Patterson syntheses based on zero layer line intensities. The determination of the halogen atomic coordinates was succeeded by three-dimensional Fourier syntheses * leading to the coordinates of the lighter atoms. Finally, a series of least-squares refinements ** was carried out in which the weight factors (W) were so chosen that for an observed structure factor $F_o \leqq FB$, $W=A1$ and for $F_o > FB$, $W=A2(F_o)^{B2}$. Here, the constants $A1$, $A2$, $B2$ and FB are such that the mean value of $W^2|F_o-F_c|^2$ remains nearly constant for the different intensity intervals. The value $B2=-0.5$ was used for tetrabromoethylene and its pyrazine adduct, the value -0.8 for the tetraiodoethylene-pyrazine compound. Anisotropic thermal damping was introduced throughout for halogen atoms, for nitrogen and carbon only in the addition compounds. In these coordinates of the pyrazine hydrogen atoms were computed assuming

* Program written by P.K. Gantzel and H. Hope, adapted for UNIVAC 1107 by H. Hope.
** Program written by P.K. Gantzel, R.A. Sparks and K.N. Trueblood, modified and adapted for UNIVAC 1107 by Chr. Rømming.

sp^2 hybridisation at the carbon atoms, and they were left unaltered during the refinement process. Each refinement started with two cycles based only on observed reflexions, followed by two further cycles in which unobserved reflexions were also included, but only those with θ-values in the region where

Table 2. Observed and calculated structure factors. The columns listed are h, k, l, F_o, and F_c.

Tetrabromoethylene. R(observed) = 7.8 %, R(total) = 13.6 %.
Observed reflexions.

0	0	2	75.2	62.4	13	0	-2	71.5	-59.7	6	1	1	34.2	-15.4	4	2	1	98.7	106.1
0	0	4	81.9	-69.4	14	0	-6	37.5	31.9	6	1	3	64.1	-66.9	4	2	4	57.0	-58.1
0	0	6	156.3	142.7	14	0	-4	38.3	-32.4	6	1	4	44.7	-47.1	5	2	-8	31.5	32.7
0	0	8	39.1	26.2	0	1	2	249.8	-251.4	7	1-10		65.9	-77.7	5	2	-6	50.7	-51.3
1	0	-8	153.1	144.3	0	1	3	114.8	-126.4	7	1	-7	30.5	34.2	5	2	-5	36.8	-38.8
1	0	-6	97.9	-90.6	0	1	4	60.9	63.3	7	1	-4	61.5	-63.5	5	2	-4	50.6	-42.7
1	0	-4	183.5	-165.6	0	1	5	76.3	-80.2	7	1	-3	37.6	37.3	5	2	-3	100.2	-112.8
1	0	4	176.0	-163.0	1	1-10		56.0	58.0	7	1	-1	68.9	70.5	5	2	-2	56.6	54.4
1	0	6	72.1	-73.0	1	1	-8	60.9	-62.9	7	1	0	96.3	-99.6	5	2	-1	68.0	-61.5
2	0-10		33.6	-32.6	1	1	-7	50.7	54.4	7	1	1	37.0	32.5	5	2	1	20.4	13.9
2	0	-8	77.7	53.0	1	1	-6	149.3	-152.0	7	1	4	79.5	79.0	5	2	3	63.1	-61.6
2	0	-4	268.4	-249.7	1	1	-5	37.2	-27.4	7	1	7	32.4	32.2	5	2	5	31.9	-36.2
2	0	-2	48.1	45.0	1	1	-3	26.1	-21.2	8	1	-6	71.9	78.6	6	2	-7	63.1	57.7
2	0	2	75.7	-90.7	1	1	1	86.5	79.8	8	1	-4	107.8	111.7	6	2	-4	50.3	-47.3
2	0	4	162.7	159.0	1	1	2	109.4	-106.3	8	1	-1	58.0	51.8	6	2	-1	53.9	57.3
2	0	6	49.2	-39.3	1	1	4	107.5	-109.4	8	1	1	53.2	-52.9	6	2	0	82.6	84.8
2	0	8	84.9	-78.0	1	1	5	84.2	86.3	8	1	4	45.4	49.7	6	2	5	43.8	45.6
2	0	10	58.9	65.2	1	1	6	52.0	49.7	9	1	-8	28.4	-22.8	7	2	-8	42.5	44.6
3	0-12		48.6	-50.4	2	1	-9	64.5	62.7	9	1	-7	62.0	-61.2	7	2	-7	36.0	29.6
3	0-10		66.1	67.9	2	1	-8	62.8	56.5	9	1	-6	31.6	-36.7	7	2	-6	29.4	-31.8
3	0	-8	74.6	70.3	2	1	-7	41.0	37.9	9	1	-5	64.7	-65.2	7	2	-5	43.7	40.4
3	0	-6	26.7	29.5	2	1	-6	84.9	-87.3	9	1	-4	61.3	68.1	7	2	-3	43.9	39.2
3	0	-4	230.9	222.4	2	1	-5	27.6	-23.6	9	1	-1	30.7	-22.1	7	2	1	28.8	-16.5
3	0	-2	28.4	-29.3	2	1	-3	69.4	64.3	9	1	0	119.4	-116.9	7	2	2	43.2	39.4
3	0	0	8.2	-4.8	2	1	-2	208.1	221.9	9	1	1	53.4	-50.4	7	2	5	29.6	34.3
3	0	2	216.6	249.5	2	1	-1	45.7	43.6	10	1	-8	84.6	-83.1	8	2	-7	41.7	-40.9
3	0	4	74.1	89.6	2	1	1	31.9	-14.3	10	1	-3	57.3	58.6	8	2	-5	34.5	-35.2
3	0	8	34.0	-30.2	2	1	2	97.8	103.3	11	1	-4	65.6	70.8	8	2	-4	53.5	-58.8
4	0-10		46.2	-46.0	2	1	3	31.3	25.2	12	1	-4	56.5	-53.5	8	2	-1	70.1	-70.9
4	0	-8	30.6	14.9	2	1	4	49.5	48.3	12	1	-3	35.8	-37.5	8	2	1	78.5	-73.4
4	0	-6	46.0	50.7	2	1	6	70.6	-68.7	12	1	2	39.6	-38.4	9	2	-5	54.7	49.7
4	0	-2	89.7	-82.1	2	1	8	81.9	76.5	14	1	-2	33.6	36.5	9	2	-3	43.8	37.6
4	0	0	265.5	-281.9	3	1-10		50.5	59.8	0	2	0	112.5	-92.0	9	2	-2	44.0	-43.9
4	0	2	41.6	44.6	3	1	-8	25.7	-28.2	0	2	1	46.0	-42.3	9	2	-1	26.1	-2.3
4	0	4	61.0	72.2	3	1	-7	37.1	-24.7	0	2	2	45.1	41.8	9	2	2	28.6	29.5
4	0	6	163.3	-156.9	3	1	-6	48.2	44.1	0	2	3	47.5	-44.1	10	2	-5	51.1	42.8
5	0-10		37.5	-40.2	3	1	-5	55.7	-49.1	0	2	4	52.1	50.6	10	2	-3	37.8	30.3
5	0	-8	160.7	-156.3	3	1	-4	45.1	-48.5	0	2	5	64.4	61.7	10	2	0	28.5	-30.4
5	0	-6	102.5	100.1	3	1	-2	102.8	-102.6	0	2	7	39.9	42.1	11	2	-3	40.0	-41.0
5	0	-4	95.1	92.4	3	1	-1	75.7	-83.0	1	2	-9	34.3	39.0	12	2	-1	31.2	37.9
5	0	-2	245.7	-263.6	3	1	0	133.1	150.7	1	2	-8	41.7	-43.7	0	3	3	25.7	22.5
5	0	2	61.2	60.9	3	1	1	106.0	-110.8	1	2	-6	44.4	44.4	0	3	5	48.9	48.7
5	0	6	32.5	39.0	3	1	3	41.4	44.1	1	2	-3	131.5	131.1	1	3	-4	31.7	-29.3
6	0-10		34.3	-35.8	3	1	4	92.0	-90.5	1	2	1	40.8	-40.6	1	3	-3	45.8	46.5
6	0	-8	66.7	44.7	3	1	6	39.9	-36.8	1	2	2	98.1	-100.2	1	3	1	21.8	-27.0
6	0	-6	114.9	114.9	3	1	7	71.7	-68.5	1	2	3	57.0	53.2	1	3	4	42.0	44.0
6	0	-4	181.9	172.3	3	1	8	29.4	-12.9	1	2	4	52.9	45.9	1	3	6	24.6	-32.7
6	0	-2	75.3	69.9	4	1	-8	35.7	36.2	1	2	5	30.3	28.4	2	3	-6	22.9	23.1
6	0	2	98.4	93.2	4	1	-7	28.6	-25.5	1	2	6	52.8	47.9	2	3	-4	57.4	51.4
6	0	8	41.9	42.4	4	1	-6	73.2	-70.0	2	2	-7	83.1	-76.0	2	3	1	26.6	-29.5
7	0-10		54.5	-57.1	4	1	-5	85.3	87.3	2	2	-6	60.1	-50.7	2	3	2	32.9	32.5
7	0	-8	90.6	-84.4	4	1	-4	75.3	-76.1	2	2	-5	31.4	-29.0	2	3	4	21.3	24.3
7	0	-6	35.3	36.1	4	1	-3	56.0	51.7	2	2	-4	98.3	96.3	3	3	-5	24.8	25.2
7	0	-4	104.1	-108.6	4	1	-2	127.6	-133.2	2	2	-3	24.3	-23.5	3	3	-4	36.9	37.7
7	0	-2	26.7	-33.9	4	1	-1	70.4	-62.6	2	2	-2	43.7	40.8	3	3	-3	37.2	38.8
7	0	2	195.7	-195.1	4	1	1	68.6	61.3	2	2	-1	60.4	-68.1	3	3	-1	27.2	31.3
7	0	6	40.0	40.1	4	1	2	123.0	129.6	2	2	0	42.9	-46.0	3	3	0	54.3	-52.1
8	0	-8	35.2	-27.8	4	1	3	91.4	92.3	2	2	1	39.0	-35.8	3	3	1	38.8	40.2
8	0	-6	119.5	-114.1	4	1	4	110.8	-106.8	2	2	3	46.6	-43.9	3	3	2	25.9	31.0
8	0	-4	39.6	40.2	4	1	6	45.8	-47.7	2	2	4	24.8	-26.6	4	3	-8	32.0	-36.3
8	0	-2	74.3	73.0	4	1	8	47.5	49.6	2	2	5	57.4	-54.7	4	3	-6	23.1	22.0
8	0	2	41.7	-40.0	5	1	-8	70.0	70.6	2	2	6	34.6	30.2	4	3	-5	46.9	-46.8
8	0	6	52.0	57.3	5	1	-7	24.2	35.3	2	2	7	37.4	-38.8	4	3	-2	31.9	-34.5
9	0-10		34.9	44.1	5	1	-6	149.5	152.7	3	2	-4	31.3	-28.9	4	3	-1	29.1	27.3
9	0	-8	43.4	50.5	5	1	-5	93.4	95.7	3	2	-2	93.0	97.5	4	3	1	29.5	-31.1
9	0	-6	29.8	-22.4	5	1	-4	104.7	-109.1	3	2	-1	31.5	-32.7	4	3	2	28.5	-31.6
9	0	-2	209.6	189.8	5	1	-3	33.8	31.6	3	2	1	69.7	77.6	5	3	-4	38.3	36.0
9	0	2	45.0	-44.7	5	1	-1	56.7	-53.3	3	2	2	69.4	-73.8	5	3	-1	32.8	33.9
9	0	4	63.2	62.5	5	1	0	148.0	165.4	3	2	3	62.8	60.1	5	3	0	25.7	21.5
10	0-10		59.0	61.7	5	1	1	34.4	29.4	3	2	4	37.8	33.6	6	3	-4	26.3	-28.7
10	0	-8	59.5	-64.9	5	1	2	25.7	28.0	3	2	5	55.7	-55.6	6	3	-3	21.3	23.8
10	0	-6	112.4	-107.6	5	1	3	27.5	25.4	3	2	9	31.8	36.9	6	3	-2	35.9	37.7
10	0	-2	54.6	-55.9	5	1	4	48.4	51.3	4	2-10		46.5	46.5	6	3	2	47.5	-46.9
10	0	0	44.7	-44.0	5	1	5	45.0	-46.7	4	2	-8	31.2	-29.2	7	3	-6	32.4	-32.5
10	0	2	39.7	-33.1	6	1-12		33.0	-42.1	4	2	-7	71.8	65.8	7	3	-3	37.3	-35.8
11	0	-6	40.8	-51.2	6	1	-9	64.6	-68.6	4	2	-6	35.0	-29.0	8	3	-2	45.6	42.5
11	0	2	69.6	61.6	6	1	-8	51.7	43.2	4	2	-5	76.4	68.3	8	3	-1	29.8	-25.9
12	0-10		40.8	40.9	6	1	-7	29.6	-27.1	4	2	-4	46.2	46.7	1	4	2	30.3	26.9
12	0	-6	74.5	71.2	6	1	-6	32.5	28.8	4	2	-3	49.4	-48.7	2	4	3	19.8	22.2
12	0	0	67.3	61.4	6	1	-3	102.7	-108.1	4	2	-1	56.6	54.7	3	4	-5	21.5	20.6
13	0	-6	35.9	-27.3	6	1	-2	117.3	-123.4	4	2	0	56.7	58.5	3	4	-2	31.2	-27.8
13	0	-4	41.8	-53.9	6	1	-1	44.8	-52.4						7	4	0	24.7	2.8

Table 2. Continued. Tetrabromoethylene. Unobserved reflexions.

0	0 10	17.4	27.1	4	1 7	15.3	-.6	11	1 -1	15.5	-27.5	7	2 4	15.0	-21.4
1	0-10	17.0	1.7	5	1-10	15.7	-31.1	11	1 0	15.9	29.0	8	2 -8	15.0	26.0
1	0 -2	7.0	1.0	5	1 -9	14.7	-8.2	11	1 1	16.3	5.6	8	2 -6	13.7	32.5
1	0 0	4.7	-.6	5	1 -2	9.8	16.2	12	1 -6	16.2	-26.7	8	2 -3	12.8	14.3
1	0 2	8.0	-2.3	5	1 6	15.0	5.4	12	1 -5	16.0	-16.1	8	2 -2	12.8	-7.0
1	0 8	15.6	-13.6	5	1 7	15.9	2.4	12	1 -2	16.2	19.2	8	2 0	13.3	8.1
1	0 10	17.8	-38.6	6	1-10	15.8	2.7	12	1 -1	16.4	-25.3	8	2 2	14.4	-16.8
2	0 -6	12.3	8.9	6	1 -5	11.8	-1.2	0	2 6	12.4	-1.7	8	2 3	15.1	18.0
3	0 6	14.4	-5.8	6	1 -4	11.3	-5.4	0	2 8	14.6	17.2	9	2 -8	15.4	3.9
4	0 -4	10.6	14.8	6	1 0	11.2	-1.8	1	2 -7	13.2	9.5	9	2 -7	14.8	-23.1
4	0 8	17.2	-19.8	6	1 2	12.4	10.4	1	2 -5	10.9	-22.3	9	2 -6	14.4	8.3
5	0 0	10.7	-7.9	6	1 5	14.8	-13.4	1	2 -4	9.6	2.9	9	2 -4	13.8	20.9
5	0 4	13.9	-9.6	6	1 6	15.7	15.5	1	2 -2	9.5	11.5	9	2 0	14.3	-1.0
6	0 0	11.8	-5.5	7	1 -9	15.1	4.1	1	2 7	13.9	-15.5	9	2 1	14.7	8.6
6	0 4	14.7	-6.5	7	1 -8	14.4	29.4	1	2 8	15.0	-34.5	10	2 -7	15.4	-4.4
6	0 6	16.6	23.6	7	1 -6	12.9	-4.7	2	2 -9	15.1	13.0	10	2 -6	15.0	18.8
7	0 0	12.9	-3.2	7	1 -5	12.4	21.3	2	2 -8	14.1	-10.0	10	2 -4	14.6	-3.5
7	0 4	15.6	-28.9	7	1 -2	11.7	23.4	2	2 2	8.7	10.7	10	2 -2	14.6	.4
8	0-10	17.1	6.2	7	1 2	13.3	-16.0	2	2 8	15.4	16.8	10	2 -1	14.8	-16.5
8	0 0	13.8	-7.0	7	1 3	14.0	-17.3	3	2 -9	15.0	1.1	11	2 -4	15.4	11.5
8	0 4	16.4	-7.3	7	1 5	15.6	28.0	3	2 -8	14.0	-10.9	0	3 1	15.6	-1.1
9	0 -4	14.3	20.3	7	1 6	16.4	-20.6	3	2 -7	12.9	-21.8	0	3 2	7.2	13.9
9	0 0	14.8	1.3	8	1-10	16.2	14.6	3	2 -6	11.9	-16.5	0	3 4	10.2	-11.8
10	0 -4	15.1	-13.6	8	1 -9	15.4	15.1	3	2 -5	10.8	-14.7	1	3 -6	12.4	-16.8
11	0 -8	17.2	9.7	8	1 -8	14.7	-27.2	3	2 -3	8.8	2.2	1	3 -5	11.2	16.9
11	0 -4	16.0	2.2	8	1 -7	14.1	17.1	3	2 0	7.9	-13.0	1	3 -2	6.9	9.1
11	0 -2	16.1	23.1	8	1 -5	13.1	-33.3	3	2 6	3.9	-7.4	1	3 2	8.0	-15.1
11	0 0	16.7	-4.0	8	1 -3	12.6	16.3	3	2 7	14.9	20.6	1	3 3	9.4	8.4
12	0 -4	16.9	-4.6	8	1 -2	12.6	-2.2	4	2 -9	14.9	5.4	1	3 5	12.0	-15.8
12	0 -2	17.1	-21.7	8	1 0	13.1	9.5	4	2 -2	8.9	-4.4	2	3 -5	11.0	3.7
0	1 6	17.2	11.6	8	1 2	14.2	12.3	4	2 2	10.7	-3.8	2	3 -3	8.6	-7.3
0	1 7	18.8	15.9	8	1 3	14.8	-30.7	4	2 3	11.6	4.0	2	3 -2	7.3	-20.9
0	1 8	14.4	-21.5	8	1 5	16.3	20.8	4	2 5	13.5	-19.0	2	3 0	6.6	6.9
0	1 9	15.4	-18.0	9	1 -9	15.8	3.7	4	2 6	14.5	27.8	2	3 3	10.2	-15.3
1	1 -9	15.1	12.5	9	1 -3	13.0	-3.0	5	2 -9	15.0	-7.3	2	3 5	12.6	12.6
1	1 -4	9.5	18.6	9	1 -2	13.5	-12.7	5	2 -7	13.2	14.0	3	3 -6	12.2	-.8
1	1 -2	11.4	-19.7	9	1 2	15.0	15.1	5	2 0	10.3	-11.6	3	3 -2	8.2	-6.7
1	1 -1	9.0	3.4	9	1 3	15.7	-18.2	5	2 2	11.7	4.8	3	3 3	11.0	-22.8
1	1 7	13.7	19.5	9	1 4	16.4	-1.3	5	2 4	13.4	-19.1	3	3 4	12.1	1.0
1	1 8	14.7	-5.4	10	1 -9	16.3	26.1	5	2 6	15.2	-30.2	4	3 -4	10.4	-17.1
1	1 9	15.8	-2.0	10	1 -7	15.2	-2.6	6	2 -9	15.1	-10.8	4	3 -3	9.7	-6.3
2	1-10	15.9	27.7	10	1 -6	14.8	16.2	6	2 -8	14.3	.0	4	3 0	9.5	4.6
2	1 -4	9.4	13.1	10	1 -5	14.5	7.7	6	2 -6	12.7	24.7	4	3 3	11.9	-29.0
2	1 0	9.0	1.9	10	1 -4	14.3	4.3	6	2 -5	12.0	-19.1	5	3 -6	12.6	2.6
2	1 5	12.0	22.3	10	1 -2	14.4	-11.6	6	2 -3	11.0	-17.8	5	3 -5	11.8	-19.4
2	1 7	14.1	-32.4	10	1 -1	14.6	18.9	6	2 -2	10.9	-18.3	5	3 -3	10.5	-17.4
2	1 9	16.2	-22.6	10	1 0	15.0	.5	6	2 2	12.6	-21.2	5	3 -2	10.2	17.4
3	1 -9	14.7	1.4	10	1 1	15.4	12.2	6	2 3	13.3	25.2	5	3 1	11.2	16.4
3	1 -3	8.6	-6.0	10	1 2	15.9	-19.8	6	2 4	14.1	-21.1	6	3 -5	12.3	-20.3
3	1 2	9.5	-7.1	11	1 -8	16.3	-5.8	7	2 -9	15.3	30.7	6	3 -1	11.3	14.9
3	1 5	12.6	-14.0	11	1 -7	15.8	-7.9	7	2 -4	12.2	-14.6	6	3 0	11.7	-3.1
4	1-10	15.7	-10.1	11	1 -6	15.5	6.5	7	2 -2	11.9	-10.4	6	3 1	12.2	14.1
4	1 -9	14.7	-1.4	11	1 -5	15.3	13.1	7	2 -1	12.0	12.9	7	3 -4	12.5	-2.2
4	1 0	9.0	-10.1	11	1 -3	15.1	-16.1	7	2 0	12.4	-.9	7	3 -2	12.2	.6
4	1 5	13.3	10.7	11	1 -2	15.3	19.0	7	2 3	14.2	6.3	7	3 -1	12.3	-10.0

Tetrabromoethylene-pyrazine. R(observed)=7.1 %, R(total)=11.1 %. Observed reflexions.

0	0 2	30.3	24.0	4	0-10	44.1	-41.5	8	0 0	67.4	-64.2	1	1 -7	59.1	59.4
0	0 4	152.4	-185.7	4	0 -8	73.3	-71.5	8	0 4	18.2	19.1	1	1 -6	87.0	-87.6
0	0 6	47.9	42.1	4	0 -6	120.0	124.1	8	0 6	18.9	-16.3	1	1 -5	79.8	-82.5
0	0 8	73.6	74.4	4	0 -4	89.6	91.1	9	0-14	35.5	-39.7	1	1 -4	23.2	-21.0
0	0 10	12.9	-11.0	4	0 -2	165.6	-186.6	9	0-12	29.9	33.3	1	1 -2	109.2	107.0
1	0-14	21.0	18.3	4	0 0	70.0	-56.1	9	0-10	41.6	45.6	1	1 -1	163.7	162.7
1	0-12	52.1	-50.1	4	0 2	102.4	120.1	9	0 -8	48.9	-49.6	1	1 1	17.5	-18.3
1	0-10	22.6	-20.4	4	0 6	41.0	-41.5	9	0 -6	38.3	-35.6	1	1 2	82.1	-89.2
1	0 -8	119.8	128.7	5	0-14	40.6	41.6	9	0 4	42.0	-48.4	1	1 3	53.7	-57.5
1	0 -6	16.7	15.1	5	0-12	40.8	40.5	9	0 8	30.3	29.8	1	1 4	53.4	-54.5
1	0 -4	148.1	-173.0	5	0-10	87.8	-91.2	10	0-14	23.4	-19.7	1	1 5	65.6	69.2
1	0 -2	32.5	26.3	5	0 -8	37.5	-41.5	10	0 -4	54.6	-54.8	1	1 6	30.1	28.6
1	0 2	39.5	-35.4	5	0 -6	129.6	135.2	10	0 -2	21.2	-14.3	1	1 8	38.3	38.6
1	0 4	14.8	3.3	5	0 -4	34.6	29.5	10	0 0	67.9	66.6	1	1 9	35.3	-34.4
1	0 8	28.5	-28.1	5	0 -2	78.0	-74.4	10	0 4	43.5	-45.7	1	1 11	26.4	24.6
1	0 10	33.3	31.9	5	0 0	17.6	18.0	11	0-12	28.0	-27.7	1	1 12	25.9	-24.2
1	0 12	29.7	30.7	5	0 6	43.5	46.0	11	0 -8	50.3	49.1	2	1-15	21.8	20.1
1	0 14	26.6	-24.9	5	0 10	39.0	-38.5	11	0 -4	65.9	-73.3	2	1-14	27.1	-24.6
2	0-16	31.9	31.9	6	0-14	39.1	40.8	11	0 0	46.6	41.6	2	1-10	44.7	46.3
2	0-12	58.5	-62.2	6	0-10	45.6	-46.4	11	0 2	29.9	-28.0	2	1 -9	48.2	48.6
2	0-10	23.7	25.1	6	0 -2	54.6	54.6	12	0-12	37.9	-44.0	2	1 -8	35.1	29.0
2	0 -8	100.0	104.9	6	0 0	47.9	-43.0	12	0 -8	48.6	51.8	2	1 -7	20.1	-15.8
2	0 -6	28.6	-25.0	6	0 2	90.3	-100.4	12	0 -4	28.6	-32.3	2	1 -6	61.7	-60.5
2	0 -4	51.9	-46.3	6	0 4	44.1	49.3	14	0 -6	24.1	22.7	2	1 -5	35.3	-34.5
2	0 -2	55.4	46.8	6	0 6	56.2	61.8	14	0 -2	28.2	-31.2	2	1 -4	60.0	-56.8
2	0 2	63.5	69.7	6	0 8	41.4	-46.6	15	0 -6	27.8	29.1	2	1 -3	99.6	95.7
2	0 4	66.7	70.1	6	0 10	27.7	-25.1	0	1 1	62.6	53.8	2	1 -2	72.6	70.5
2	0 6	81.8	-90.4	7	0-10	32.1	32.4	0	1 2	110.5	-119.4	2	1 -1	10.4	-9.5
2	0 8	48.2	-48.4	7	0 -8	18.5	-17.6	0	1 3	81.9	-81.9	2	1 0	113.6	118.3
2	0 10	64.9	66.3	7	0 -6	89.1	-93.1	0	1 4	15.1	-12.1	2	1 1	85.4	-97.0
2	0 14	31.4	-29.5	7	0 -4	53.6	52.4	0	1 5	27.7	25.8	2	1 3	66.1	74.1
3	0-16	27.5	27.2	7	0 -2	118.7	121.9	0	1 6	75.3	73.3	2	1 4	68.8	-78.7
3	0-12	26.4	-22.7	7	0 0	78.9	-76.7	0	1 7	67.8	67.6	2	1 5	48.9	50.6
3	0 -8	14.4	-15.4	7	0 2	78.5	-85.9	0	1 8	26.5	26.2	2	1 7	53.4	-55.5
3	0 -6	68.3	62.7	7	0 4	46.6	50.3	0	1 9	34.8	-32.7	2	1 8	49.1	53.9
3	0 -4	108.7	109.9	7	0 8	27.8	-28.0	0	1 10	24.4	-23.1	2	1 11	30.5	31.6
3	0 -2	126.8	-140.2	8	0-14	30.6	-34.3	0	1 11	15.4	-14.5	2	1 12	24.9	-22.4
3	0 0	119.5	-122.3	8	0-12	18.7	19.6	0	1 12	14.2	-16.0	3	1-14	20.8	-19.6
3	0 2	141.8	191.5	8	0-10	60.0	65.9	0	1 13	28.4	27.1	3	1-13	19.8	-18.0
3	0 4	72.0	79.5	8	0 -8	58.4	-59.4	1	1-14	23.3	-19.1	3	1-12	22.8	-21.5
3	0 6	99.2	-111.5	8	0 -6	88.1	-90.8	1	1-11	34.6	-34.3	3	1-11	39.2	39.3
3	0 10	49.6	49.7	8	0 -4	69.0	70.8	1	1-10	52.0	51.7	3	1-10	25.9	24.6
4	0-12	38.9	37.5	8	0 -2	41.5	42.7	1	1 -9	35.6	34.8	3	1 -9	18.8	20.4

Table 2. Continued. Tetrabromoethylene-pyrazine.

3	1 -8	50.4	48.8	8	1 -8	49.3	-49.8	3	2 -1	16.2	14.1	1	3 8	29.2	-28.9
3	1 -7	64.9	-64.3	8	1 -7	55.7	-53.7	3	2 0	50.1	-48.3	1	3 9	22.6	-21.2
3	1 -6	15.9	-12.6	8	1 -6	22.3	22.2	3	2 1	40.9	41.7	2	3 -9	31.6	30.1
3	1 -5	42.4	37.0	8	1 -4	57.1	54.3	3	2 5	21.4	-20.3	2	3 -8	27.7	-26.1
3	1 -4	93.4	-90.5	8	1 -3	49.7	46.2	3	2 7	16.7	15.4	2	3 -7	17.0	-15.3
3	1 -3	81.2	78.6	8	1 -2	20.3	-19.4	3	2 8	29.3	30.2	2	3 -6	26.6	24.1
3	1 -2	36.3	-34.8	8	1 -1	44.9	-40.6	3	2 12	31.2	-26.8	2	3 -5	24.7	-22.8
3	1 -1	80.0	-75.0	8	1 0	52.0	-47.4	4	2-14	30.5	-29.2	2	3 -4	51.1	51.6
3	1 0	84.4	83.9	8	1 1	23.6	-21.6	4	2-12	27.4	29.2	2	3 -3	50.6	48.8
3	1 2	33.6	36.7	8	1 3	28.5	29.9	4	2-10	40.9	41.3	2	3 -2	29.2	-29.5
3	1 3	70.6	77.4	8	1 4	20.2	22.1	4	2 -8	32.4	-29.5	2	3 -1	14.1	12.5
3	1 4	59.4	-64.2	9	1-12	29.7	32.6	4	2 -7	24.1	22.9	2	3 0	49.4	-49.9
3	1 5	39.6	-40.9	9	1-11	20.1	21.4	4	2 -6	26.5	-21.4	2	3 1	36.3	-41.3
3	1 6	26.3	-27.5	9	1 -9	24.4	-24.8	4	2 -5	15.9	11.2	2	3 2	27.9	30.8
3	1 7	30.1	-32.4	9	1 -8	36.2	-40.7	4	2 -4	5.8	3.6	2	3 3	19.8	20.0
3	1 8	33.4	33.2	9	1 -7	19.6	-17.5	4	2 -3	29.5	-30.2	2	3 4	35.6	34.5
3	1 9	38.6	37.3	9	1 -5	42.6	40.6	4	2 -2	13.6	1.5	2	3 5	24.7	23.9
3	1 10	21.1	17.1	9	1 -4	37.7	44.2	4	2 -1	17.6	-5.0	2	3 7	22.8	-23.4
4	1-12	29.8	-31.0	9	1 -3	24.1	-21.0	4	2 0	64.1	60.5	3	3-12	23.4	22.7
4	1-11	32.3	30.0	9	1 -2	21.8	12.6	4	2 1	17.4	14.8	3	3-11	20.3	19.3
4	1 -9	47.6	-48.1	9	1 -1	44.0	-42.7	4	2 2	15.7	15.2	3	3 -8	39.2	-40.0
4	1 -8	69.4	67.7	9	1 0	25.9	-23.4	4	2 4	65.8	-75.9	3	3 -7	32.7	-32.0
4	1 -6	42.7	38.6	9	1 1	35.2	35.9	4	2 8	50.8	55.0	3	3 -6	27.7	26.5
4	1 -5	98.3	97.3	9	1 2	23.4	-18.4	4	2 12	25.4	-24.0	3	3 -4	53.4	55.8
4	1 -4	87.1	-83.8	9	1 5	30.9	-31.5	5	2 -8	35.7	35.6	3	3 -3	32.4	32.2
4	1 -3	36.7	-34.9	10	1-12	25.2	26.6	5	2 -7	22.4	18.5	3	3 -2	17.9	-18.3
4	1 -2	42.4	-41.4	10	1-10	8.5	7.8	5	2 -6	17.2	13.0	3	3 -1	29.4	-25.4
4	1 -1	78.0	-71.6	10	1 -9	27.5	-29.5	5	2 -5	8.4	-8.3	3	3 0	43.0	-40.3
4	1 0	100.9	95.0	10	1 -8	29.5	-30.3	5	2 -4	96.5	-92.6	3	3 3	28.9	30.1
4	1 1	79.8	84.5	10	1 -7	20.8	20.1	5	2 -1	31.6	26.5	3	3 4	25.0	25.4
4	1 2	53.3	53.5	10	1 -6	26.9	-25.5	5	2 0	117.1	109.3	3	3 6	19.8	18.9
4	1 3	16.4	16.5	10	1 -4	17.7	17.3	5	2 2	17.8	-15.6	4	3-12	28.8	25.7
4	1 4	42.1	-43.9	10	1 -3	44.1	-43.9	5	2 4	79.9	-81.4	4	3 -8	28.9	-29.4
4	1 5	53.1	-59.1	10	1 -2	32.5	30.0	5	2 8	30.2	28.6	4	3 -5	30.4	25.5
4	1 6	36.4	-35.1	10	1 1	24.2	23.7	6	2-12	38.4	-36.1	4	3 -4	29.6	25.9
4	1 7	24.5	24.6	10	1 2	26.5	-24.3	6	2 -8	82.1	81.1	4	3 -3	20.7	-21.0
4	1 9	24.2	21.7	10	1 3	30.4	-30.8	6	2 -6	6.3	-4.8	4	3 -2	25.1	26.7
4	1 10	19.4	18.2	11	1-11	26.8	-28.0	6	2 -4	102.2	-100.5	4	3 -1	24.0	-20.7
4	1 11	27.0	-23.7	11	1-10	26.2	24.7	6	2 -2	25.4	23.8	4	3 1	32.2	32.9
5	1-13	30.4	32.1	11	1 -7	29.7	33.2	6	2 0	73.4	69.0	4	3 2	33.6	-34.1
5	1-12	35.3	-35.4	11	1 -6	34.0	-34.5	6	2 2	29.3	-27.0	4	3 5	28.0	-29.5
5	1-10	36.1	-36.5	11	1 -5	24.4	-24.9	6	2 3	21.2	21.5	4	3 6	31.8	33.9
5	1 -9	40.4	-41.1	11	1 -3	21.8	-22.2	6	2 4	16.4	-20.3	5	3 -9	16.3	-11.8
5	1 -8	52.7	51.4	11	1 -2	31.1	31.3	7	2-12	48.5	-51.0	5	3 -7	31.1	31.1
5	1 -7	44.8	42.5	11	1 -1	29.6	29.1	7	2 -8	63.5	59.6	5	3 -6	24.6	-21.9
5	1 -6	60.3	62.2	11	1 2	20.9	-23.5	7	2 -7	20.0	-20.2	5	3 -3	38.4	-35.8
5	1 -5	17.9	18.3	12	1-13	10.5	-9.1	7	2 -6	23.3	-21.4	5	3 -2	47.8	45.6
5	1 -4	49.8	-48.1	12	1-10	23.8	27.3	7	2 -4	42.5	-42.7	5	3 -1	27.2	24.0
5	1 -3	82.4	-77.4	12	1 -9	19.0	16.9	7	2 -3	17.1	19.0	5	3 1	29.8	29.1
5	1 -2	77.7	-74.9	12	1 -6	27.3	-28.1	7	2 -1	19.1	-14.0	5	3 2	38.6	-40.8
5	1 -1	29.9	25.5	12	1 -5	25.8	-26.5	7	2 4	17.7	20.0	5	3 3	27.9	-29.2
5	1 0	22.6	17.8	12	1 -3	20.3	18.2	7	2 6	22.9	-25.3	5	3 6	27.4	28.2
5	1 1	45.9	42.6	12	1 -2	25.1	20.1	8	2-12	27.7	-24.4	5	3 7	19.7	20.1
5	1 2	57.6	62.3	12	1 1	23.7	-24.7	8	2 -6	17.5	12.4	6	3-11	20.1	-23.0
5	1 3	54.9	-60.0	0	2 0	29.0	7.4	8	2 -5	23.6	21.6	6	3-10	32.2	31.9
5	1 4	14.2	15.3	0	2 1	31.5	-27.7	8	2 -4	24.2	21.2	6	3 -7	27.9	26.3
5	1 6	26.3	-29.3	0	2 2	30.3	-30.3	8	2 -2	47.7	-45.5	6	3 -6	45.7	-48.8
5	1 7	38.6	36.3	0	2 3	14.6	-11.7	8	2 0	48.3	-39.3	6	3 -5	31.0	-29.2
5	1 9	23.5	-22.8	0	2 4	16.1	13.2	8	2 2	55.1	48.4	6	3 -3	19.7	-19.2
5	1 10	20.0	17.0	0	2 5	29.5	25.3	8	2 6	40.0	-40.9	6	3 -2	52.5	56.7
6	1-11	36.6	-34.1	0	2 6	72.4	70.2	9	2-10	26.8	-27.7	6	3 -1	34.9	26.2
6	1-10	36.5	-36.7	0	2 8	25.6	-21.9	9	2 -9	8.5	-9.3	6	3 2	30.3	-30.2
6	1 -8	20.5	19.7	0	2 9	12.8	-14.5	9	2 -8	32.1	-30.0	6	3 3	20.5	-18.6
6	1 -7	47.0	46.2	0	2 10	46.9	-47.3	9	2 -6	45.9	49.0	7	3-10	31.5	32.3
6	1 -6	56.8	54.5	0	2 12	28.8	26.2	9	2 -4	29.1	28.6	7	3 -6	32.6	-30.5
6	1 -5	55.5	-54.5	0	2 14	24.8	22.9	9	2 -2	64.6	-63.5	7	3 -3	21.9	19.4
6	1 -3	13.0	-14.0	1	2-14	24.5	24.1	9	2 0	19.5	-14.9	7	3 -2	23.1	19.0
6	1 -2	56.1	-53.9	1	2-10	20.1	-18.5	9	2 2	47.5	42.1	7	3 1	25.3	-24.5
6	1 -1	78.1	77.6	1	2 -5	17.1	-17.5	10	2-10	41.5	-46.1	8	3-10	24.2	21.4
6	1 0	29.0	-28.0	1	2 -4	30.8	27.7	10	2 -6	50.2	49.3	8	3 -8	9.8	9.8
6	1 1	32.5	-31.7	1	2 -3	27.7	21.8	10	2 -2	44.6	-40.3	8	3 -7	21.7	-21.1
6	1 2	40.0	38.0	1	2 -2	100.2	98.4	11	2-10	25.2	-28.0	8	3 -1	32.9	-27.5
6	1 3	44.2	-49.6	1	2 -1	18.1	13.4	11	2 2	27.0	-24.8	8	3 0	27.6	24.6
6	1 4	26.7	28.0	1	2 2	99.7	-110.8	12	2 -6	24.9	-25.4	8	3 3	28.3	22.6
6	1 5	37.6	38.5	1	2 3	14.6	12.0	12	2 -2	30.5	26.6	8	3 4	22.8	-20.3
6	1 6	26.6	-25.5	1	2 4	70.5	73.7	13	2 -6	26.2	-25.6	9	3 -9	19.3	-20.7
6	1 8	23.0	-20.7	1	2 6	83.9	87.7	13	2 -4	27.2	23.6	9	3 -8	21.8	22.0
6	1 9	27.9	-27.8	1	2 8	52.0	-49.7	0	3 1	25.6	27.7	9	3 -6	18.5	14.6
7	1-14	24.8	23.8	1	2 10	35.1	-31.8	0	3 2	29.7	31.1	9	3 -5	26.7	24.7
7	1-10	38.2	-39.0	1	2 12	29.4	24.9	0	3 3	26.6	-25.5	9	3 -4	30.7	-28.3
7	1 -9	43.7	41.9	2	2-10	44.1	43.1	0	3 4	23.8	23.4	9	3 -1	28.6	-24.2
7	1 -8	21.1	-19.4	2	2 -6	97.8	-96.6	0	3 5	12.9	12.2	9	3 0	30.4	25.9
7	1 -7	22.7	-22.7	2	2 -4	62.5	56.7	0	3 6	28.3	-28.0	10	3-10	9.6	-12.1
7	1 -6	59.7	54.5	2	2 -2	137.7	138.0	0	3 7	28.2	24.7	10	3 -8	19.8	22.9
7	1 -5	55.3	-55.8	2	2 -1	28.1	-26.7	0	3 8	25.5	-25.4	10	3 -4	22.5	-23.8
7	1 -4	57.8	52.7	2	2 0	77.8	-74.1	0	3 9	17.2	-17.2	11	3-11	7.5	-7.3
7	1 -3	51.2	48.3	2	2 2	75.6	-87.2	0	3 10	21.9	21.7	0	4 0	42.1	46.6
7	1 -2	46.7	-42.1	2	2 3	16.4	14.1	0	3 12	17.2	16.7	0	4 4	34.2	-34.9
7	1 0	55.0	-49.0	2	2 4	63.6	66.4	1	3-10	18.1	-13.9	0	4 8	17.8	17.5
7	1 1	65.7	-64.5	2	2 6	34.5	34.3	1	3 -6	24.9	21.4	1	4 -8	31.1	32.4
7	1 2	33.2	33.9	2	2 8	24.3	-19.2	1	3 -5	33.2	-31.0	1	4 -4	35.1	-38.8
7	1 3	23.5	22.0	3	2-14	27.8	-26.2	1	3 -4	22.8	20.9	1	4 -3	12.2	12.1
7	1 4	40.6	39.5	3	2-12	23.9	20.9	1	3 -2	30.9	-29.2	1	4 -1	7.7	-8.6
7	1 5	29.5	30.1	3	2-10	62.7	65.7	1	3 -1	41.7	39.8	1	4 3	13.9	15.2
7	1 7	29.3	-32.5	3	2 -8	46.4	-43.4	1	3 1	26.5	-32.5	2	4 -8	18.8	21.4
8	1-13	23.9	-25.0	3	2 -6	77.7	-74.4	1	3 2	31.0	35.8	2	4 -5	10.5	13.5
8	1-12	26.1	26.2	3	2 -5	17.5	15.4	1	3 3	19.8	-20.1	2	4 -1	13.6	-16.6
8	1-11	24.9	23.7	3	2 -4	84.8	77.0	1	3 4	46.7	53.2	2	4 2	15.9	18.0
8	1-10	27.8	-25.0	3	2 -3	19.9	-11.7	1	3 5	37.3	41.2	2	4 3	15.9	19.6
8	1 -9	19.8	19.6	3	2 -2	66.4	58.6	1	3 6	23.3	-23.4	2	4 4	17.9	16.6

Table 2. Continued. Tetrabromoethylene-pyrazine.

2	4	6	21.5	-20.1	4	4	-4	18.4	19.4	6	4	2	21.8	-22.5	0	5	3	7.7	-10.7
3	4	-6	15.7	15.0	4	4	-2	35.5	-37.1	7	4	-6	22.7	-21.7	0	5	6	9.0	11.1
3	4	-5	12.8	12.9	4	4	0	17.0	-10.8	7	4	-4	16.1	15.1	1	5	-6	17.8	-16.9
3	4	-4	16.3	15.0	4	4	2	21.2	27.3	7	4	-2	25.1	22.4	1	5	-2	12.2	18.1
3	4	-2	27.9	-28.5	5	4	-6	23.0	26.3	7	4	0	19.2	-20.7	1	5	-1	6.7	8.1
3	4	0	17.6	-18.4	5	4	-5	10.9	-14.7	8	4	-8	17.8	-16.8	3	5	0	14.6	16.9
3	4	2	31.7	36.2	5	4	-2	17.4	-17.2	8	4	-6	21.0	-20.6	4	5	-4	17.1	-14.8
3	4	6	24.0	-26.0	5	4	-1	22.1	20.8	8	4	-4	17.6	18.3	4	5	0	16.7	16.7
4	4	-6	31.5	33.7	6	4	-2	16.2	16.2	0	5	2	16.4	-19.4					

Unobserved reflexions

0	0	12	4.0	-1.6	11	1	-4	9.6	2.0	7	2	0	8.6	-6.1	6	3	1	8.4	-10.1
1	0	6	9.1	10.1	11	1	0	10.2	-2.0	7	2	1	8.7	-8.7	6	3	4	8.4	-2.7
2	0	0	5.5	5.7	11	1	1	10.4	-4.7	7	2	2	8.7	6.8	6	3	5	8.7	15.1
3	0	10	8.2	-3.6	11	1	3	10.9	-19.8	7	2	3	8.7	9.8	7	3	-9	8.5	17.2
3	0	8	8.4	-8.5	11	1	4	11.0	-4.2	7	2	5	8.9	-4.1	7	3	-8	8.1	7.4
4	0	4	6.6	-5.3	11	1	5	11.1	13.1	8	2	11	9.2	11.3	7	3	-7	3.4	-.5
4	0	8	8.8	6.9	12	1	-8	9.7	3.3	8	2	10	8.8	1.1	7	3	-5	8.9	-15.4
4	0	10	9.8	-12.0	12	1	-7	9.7	-5.3	8	2	-9	8.4	-7.9	7	3	-4	7.6	-4.2
5	0	2	6.9	-3.0	12	1	-4	10.2	-5.5	8	2	-8	3.3	3.6	7	3	-1	8.8	1.6
5	0	4	7.2	-7.2	12	1	-1	10.4	9.5	8	2	-7	7.9	-5.3	7	3	0	9.0	9.7
5	0	8	9.1	-11.7	12	1	0	10.5	8.9	8	2	-3	8.3	4.7	7	3	2	9.1	.5
6	0	12	9.2	19.9	13	1	-7	10.3	-18.5	8	2	-1	9.0	-10.5	7	3	3	9.0	9.4
6	0	-8	7.3	-13.9	13	1	-6	10.3	-15.6	8	2	1	9.3	9.0	7	3	4	9.1	-11.1
6	0	-6	6.9	-3.6	13	1	-5	10.5	2.4	8	2	3	9.4	4.6	8	3	-9	8.8	-1.9
6	0	-4	6.4	-2.2	13	1	-4	10.7	-14.1	8	2	4	9.4	17.0	8	3	-6	8.1	-10.0
7	0	12	9.3	4.8	13	1	-3	10.7	17.7	8	2	5	9.5	-5.7	8	3	-5	8.1	11.9
7	0	6	8.9	16.8	0	2	7	3.5	-4.3	9	2	11	9.4	8.7	8	3	-4	8.3	-16.2
8	0	2	9.0	-1.8	0	2	11	4.0	3.6	9	2	-7	8.3	-4.9	8	3	-3	8.7	15.3
9	0	-4	8.4	16.8	1	2	11	9.3	-3.3	9	2	-5	8.4	.8	8	3	-2	9.0	-2.4
9	0	-2	8.9	-7.0	1	2	-9	8.3	13.3	9	2	-3	8.9	-7.0	8	3	1	9.7	-4.1
9	0	0	9.2	12.1	1	2	-8	7.8	.9	9	2	-1	9.4	3.4	8	3	2	9.7	10.2
9	0	2	9.6	2.7	1	2	-7	7.2	-9.8	9	2	1	9.8	4.4	9	3	-7	8.7	-9.6
10	0	12	9.6	6.4	1	2	-6	6.6	-7.2	9	2	3	10.0	-7.6	9	3	-3	9.3	-8.6
10	0	10	3.4	1.8	1	2	1	4.7	-7.7	9	2	4	10.1	-5.4	9	3	-2	9.7	-16.3
10	0	-8	8.6	14.7	1	2	5	6.4	3.5	10	2	-9	9.0	4.7	9	3	1	10.2	11.4
10	0	-6	8.6	12.2	1	2	7	7.7	-3.9	10	2	-8	8.9	-20.4	10	3	-7	9.2	8.4
10	0	2	10.2	-2.6	1	2	9	8.7	11.8	10	2	-7	8.8	8.1	10	3	-6	9.2	14.1
11	0	10	9.3	-7.4	1	2	11	9.7	3.9	10	2	-5	9.0	-8.8	10	3	-5	9.4	9.9
11	0	-6	9.2	-12.8	2	2	12	9.7	4.5	10	2	-4	9.3	.4	10	3	-3	9.9	-14.7
11	0	-2	9.9	16.7	2	2	11	9.2	7.9	10	2	-3	9.5	-2.5	10	3	-2	10.2	-10.8
12	0	10	9.7	6.7	2	2	-9	8.1	9.7	10	2	-1	9.9	12.2	10	3	-1	10.3	3.8
12	0	-6	9.7	-15.4	2	2	-8	7.5	-14.9	10	2	0	10.0	2.7	0	4	1	3.4	-7.0
12	0	-2	10.3	14.2	2	2	-7	7.0	-10.8	10	2	1	10.2	-5.3	0	4	2	3.4	-2.4
12	0	0	10.5	.4	2	2	-5	5.8	5.9	10	2	2	10.5	4.2	0	4	3	3.7	2.6
13	0	-8	10.1	4.5	2	2	-3	4.4	6.8	11	2	-9	9.5	10.1	0	4	5	3.9	9.9
13	0	-6	10.3	-5.3	2	2	1	4.4	-1.7	11	2	-8	9.4	-5.2	0	4	6	3.9	6.7
13	0	-4	10.6	11.6	2	2	5	6.7	-9.5	11	2	-7	9.4	-1.6	1	4	-7	8.0	-4.3
13	0	-2	10.7	-9.5	2	2	7	7.9	1.0	11	2	-6	9.5	9.4	1	4	-6	7.3	-.3
1	1	12	9.6	4.5	2	2	9	9.0	8.7	11	2	-5	9.7	-13.8	1	4	-5	6.6	.3
1	1	-8	7.6	7.1	2	2	10	9.5	2.0	11	2	-4	9.8	-1.0	1	4	-2	4.0	8.2
1	1	-3	6.1	-2.7	3	2	11	9.1	3.3	11	2	-3	10.1	4.5	1	4	1	3.7	-9.6
1	1	7	7.5	2.1	3	2	-9	8.0	-4.8	11	2	-2	10.2	13.0	1	4	2	4.7	.0
1	1	10	9.0	-6.4	3	2	-7	6.9	7.7	11	2	-1	10.3	7.4	1	4	4	6.5	-8.7
2	1	13	10.0	-17.4	3	2	2	5.5	-8.9	11	2	0	10.4	-4.6	1	4	5	7.2	.0
2	1	12	9.5	-10.8	3	2	3	5.9	-8.2	12	2	-7	9.9	-5.8	1	4	6	7.9	-4.2
2	1	11	9.0	-12.3	3	2	4	6.4	-2.9	12	2	-5	10.2	-6.1	2	4	-7	7.8	-11.7
2	1	2	5.5	-.3	3	2	6	7.6	-12.0	12	2	-4	10.4	11.3	2	4	-6	7.2	.2
2	1	6	8.5	-8.8	3	2	9	9.3	9.3	12	2	-3	10.6	3.8	2	4	-5	6.4	14.7
2	1	9	8.8	7.2	3	2	10	9.8	6.4	1	3	-9	8.7	11.7	2	4	-4	5.7	-9.6
2	1	10	9.3	14.4	4	2	11	9.0	-8.3	1	3	-8	8.1	5.1	2	4	-2	3.4	-5.5
3	1	1	5.4	-1.8	4	2	-9	8.0	-12.2	1	3	-7	7.5	14.4	2	4	0	5.4	-6.1
4	1	13	9.8	12.8	4	2	3	6.5	-2.7	1	3	-3	4.7	6.4	2	4	1	4.9	2.0
4	1	10	8.3	-5.3	4	2	5	7.4	6.2	1	3	7	8.0	.7	2	4	5	7.5	-1.6
4	1	7	6.7	-8.5	4	2	6	7.9	.9	2	3	10	9.1	-13.4	3	4	-3	3.4	-.9
4	1	8	8.8	10.1	4	2	7	8.5	8.8	2	3	6	7.6	-11.7	3	4	-7	7.7	-6.5
5	1	11	8.7	-1.8	4	2	9	9.6	-4.0	2	3	8	8.8	-10.7	3	4	-1	5.7	-6.4
5	1	5	7.6	-3.1	5	2	12	9.5	2.0	3	3	-9	8.3	11.3	3	4	1	6.2	9.1
5	1	8	9.2	-13.1	5	2	11	9.0	-9.3	3	3	-5	6.0	9.5	3	4	3	6.5	-1.1
6	1	13	9.7	12.1	5	2	10	8.5	.2	3	3	1	5.8	-2.9	3	4	4	7.1	13.6
6	1	12	9.3	-19.4	5	2	-9	8.0	3.4	3	3	2	5.8	4.2	3	4	5	7.8	-4.5
6	1	-9	7.8	12.2	5	2	-3	6.0	.5	3	3	5	7.3	-11.8	4	4	-7	7.7	6.3
6	1	-4	6.4	4.5	5	2	-2	6.4	-11.4	3	3	7	8.5	-7.3	4	4	-5	6.5	5.5
6	1	7	9.0	2.9	5	2	1	7.3	-2.9	3	3	8	9.1	-6.1	4	4	-3	5.9	-2.3
7	1	13	9.8	-19.0	5	2	3	7.2	-11.3	4	3	-10	8.8	-6.4	4	4	-1	6.9	9.9
7	1	12	9.3	.2	5	2	5	7.8	6.5	4	3	-9	8.3	-9.9	4	4	1	7.3	4.0
7	1	11	8.9	-11.2	5	2	6	8.3	18.5	4	3	-7	7.2	-1.6	4	4	3	7.2	-7.0
7	1	-1	8.2	7.4	5	2	7	8.8	-2.0	4	3	-6	6.7	.9	4	4	4	7.6	3.3
7	1	6	9.0	-9.6	6	2	11	9.0	-8.3	4	3	0	7.1	-3.2	5	4	-7	7.7	3.4
8	1	-5	7.6	3.2	6	2	10	8.5	-4.4	4	3	3	6.8	-4.8	5	4	-4	6.7	5.8
8	1	2	9.1	.6	6	2	-9	8.0	3.0	4	3	4	7.2	2.4	5	4	-3	6.7	4.8
8	1	5	9.3	-18.9	6	2	-7	7.2	3.5	4	3	7	8.9	13.3	5	4	0	8.4	-4.3
8	1	6	9.5	5.5	6	2	-5	6.6	3.4	5	3	10	8.9	8.1	5	4	1	8.2	-6.1
9	1	10	8.8	-10.3	6	2	-3	6.8	13.7	5	3	-8	7.8	-8.7	5	4	2	8.0	-1.8
9	1	-6	8.1	8.1	6	2	-1	7.7	-7.2	5	3	-5	3.3	4.2	5	4	3	8.0	-7.8
9	1	3	9.7	10.9	6	2	1	8.0	-9.5	5	3	-4	6.3	9.8	6	4	-6	3.4	1.2
9	1	4	9.8	9.0	6	2	5	8.3	10.8	5	3	0	7.8	-4.6	6	4	-5	7.4	-10.8
10	1	11	9.4	-5.2	6	2	6	8.7	7.7	5	3	4	7.7	9.9	6	4	-4	7.3	7.8
10	1	-5	8.8	8.5	6	2	7	9.2	-9.7	5	3	5	8.1	-5.0	6	4	-3	7.5	9.4
10	1	-1	9.6	8.9	7	2	11	9.1	12.6	6	3	-9	8.4	8.3	6	4	-1	8.7	5.6
10	1	0	9.8	-8.2	7	2	10	8.6	6.4	6	3	-8	7.9	2.0	6	4	0	9.0	-10.5
10	1	4	10.4	4.7	7	2	-9	8.2	1.8	6	3	-4	6.9	1.0	6	4	1	9.0	-8.5
11	1	-9	9.2	2.3	7	2	-5	7.2	5.7	6	3	0	8.5	5.5	7	4	-3	8.4	8.8
11	1	-8	9.1	-7.9	7	2	-2	7.9	8.1						7	4	-1	9.4	-.3

Table 2. Continued. Tetraiodoethylene-pyrazine. R(observed) = 6.9 %, R(total) = 10.0 %. Observed reflexions.

0 0 4	179.0	-168.5	8 0-18	39.7	-32.4
0 0 6	33.2	20.1	8 0-16	38.8	-37.7
0 0 8	50.6	-52.3	8 0-10	111.1	121.1
0 0 10	109.7	115.5	8 0 -6	216.3	-207.3
0 0 12	62.8	66.8	8 0 -4	42.5	40.7
0 0 14	84.6	-92.1	8 0 -2	62.8	48.4
1 0-18	54.3	51.0	8 0 2	63.5	69.2
1 0-14	60.4	-60.0	8 0 4	121.5	-120.6
1 0-12	46.7	41.8	8 0 6	54.3	-47.9
1 0-10	23.8	-19.3	8 0 8	69.8	77.9
1 0 -8	116.2	116.7	9 0-14	67.3	-72.0
1 0 -6	85.7	82.7	9 0-10	136.2	138.7
1 0 -4	342.4	-320.1	9 0 -8	46.2	-38.7
1 0 2	19.7	-11.7	9 0 -6	55.3	-57.9
1 0 4	138.6	127.8	9 0 -2	72.9	-89.0
1 0 6	139.3	-140.0	9 0 0	111.0	115.5
1 0 8	121.3	-120.4	9 0 2	56.6	53.2
1 0 10	124.6	134.5	9 0 4	99.4	-109.4
2 0-18	39.2	41.1	10 0-18	52.5	44.4
2 0-12	58.9	-65.8	10 0-14	74.7	-98.2
2 0-10	42.6	-39.4	10 0-10	47.9	44.7
2 0 -8	246.2	243.2	10 0 -6	67.4	70.5
2 0 -6	23.9	-9.6	10 0 -4	125.8	-127.5
2 0 -4	184.6	-168.6	10 0 -2	63.7	-77.4
2 0 -2	74.5	63.7	10 0 0	113.6	122.5
2 0 0	97.5	-79.5	10 0 8	60.4	-56.2
2 0 2	214.1	190.0	11 0-18	59.5	52.9
2 0 4	176.4	166.2	11 0-14	34.9	-27.6
2 0 6	199.4	-200.4	11 0-10	64.5	-71.9
2 0 8	25.5	-22.6	11 0 -8	79.6	85.0
2 0 10	47.3	42.0	11 0 -6	66.7	74.8
2 0 14	54.8	52.5	11 0 -4	107.6	-116.3
3 0-16	49.6	45.8	11 0 4	69.0	73.5
3 0-14	51.7	48.7	11 0 6	39.3	-36.9
3 0-12	129.3	-141.4	11 0 8	39.6	-42.2
3 0-10	22.8	-6.0	12 0-14	45.1	38.4
3 0 -8	137.8	133.8	12 0-12	60.3	-62.0
3 0 -6	31.2	22.9	12 0-10	63.7	-64.0
3 0 -4	161.1	143.8	12 0 -8	82.0	86.7
3 0 -2	218.7	-193.0	12 0 0	76.5	-83.1
3 0 0	261.5	-240.6	12 0 2	39.2	38.3
3 0 2	287.6	278.9	12 0 4	56.0	55.8
3 0 4	71.4	74.1	12 0 6	36.5	-32.5
3 0 6	57.5	-52.8	13 0-16	36.1	36.3
3 0 10	92.4	-99.5	13 0-14	52.0	46.8
3 0 12	33.7	28.0	13 0-12	61.2	-65.6
3 0 14	61.2	64.2	13 0 -4	71.3	85.0
4 0-16	77.7	85.1	13 0 -2	44.8	-40.1
4 0-12	59.5	-70.8	13 0 0	66.4	-72.0
4 0 -8	91.2	-93.4	13 0 2	41.0	37.0
4 0 -6	122.7	122.8	14 0-18	42.0	-33.7
4 0 -4	252.6	229.3	14 0-16	37.0	31.3
4 0 -2	272.4	-244.0	14 0 -8	71.5	-79.0
4 0 0	96.8	-90.3	14 0 -4	64.7	70.6
4 0 2	42.5	41.3	14 0 6	45.0	43.9
4 0 4	37.7	-28.3	15 0-12	58.1	53.8
4 0 6	133.5	134.4	15 0 -8	62.3	-61.2
4 0 8	45.0	-38.3	15 0 2	41.8	-45.6
4 0 10	102.8	-111.9	16 0-16	48.3	-40.4
4 0 12	43.5	42.5	16 0-12	49.8	47.9
5 0-20	43.8	-44.1	16 0 -2	55.3	51.7
5 0-16	51.4	50.3	17 0-16	40.3	-31.9
5 0-12	63.5	69.2	17 0 -6	39.6	-43.1
5 0-10	71.0	-75.0	0 1 1	115.8	115.7
5 0 -8	162.1	-162.8	0 1 2	237.2	-241.3
5 0 -6	208.8	205.1	0 1 3	119.7	-114.3
5 0 -4	107.6	102.8	0 1 4	27.9	14.3
5 0 -2	56.6	-55.4	0 1 5	79.1	73.2
5 0 0	44.2	28.2	0 1 6	35.6	36.5
5 0 2	162.8	-168.7	0 1 8	59.7	59.9
5 0 4	43.7	41.1	0 1 9	41.1	-36.3
5 0 6	151.9	160.5	0 1 10	51.0	53.6
5 0 8	61.0	-69.4	0 1 11	57.2	61.7
6 0-16	41.9	-38.7	0 1 12	78.0	-86.0
6 0-14	49.3	41.9	0 1 13	26.1	-23.5
6 0-12	108.1	122.0	0 1 14	32.8	-27.6
6 0-10	122.3	-117.0	0 1 15	12.0	-17.0
6 0 -8	72.1	-80.3	0 1 16	43.8	39.3
6 0 -6	41.1	37.9	1 1-16	52.0	-52.8
6 0 -4	39.6	-27.2	1 1-15	33.7	-30.5
6 0 -2	184.1	181.8	1 1-14	34.5	28.6
6 0 0	47.9	-44.1	1 1-13	39.5	32.2
6 0 2	230.9	-227.7	1 1-12	40.3	36.7
6 0 4	56.0	63.6	1 1-10	23.5	24.5
6 0 6	38.1	29.1	1 1 -9	53.1	-57.2
6 0 10	35.5	33.6	1 1 -7	94.0	99.0
6 0 12	59.4	-65.3	1 1 -6	188.1	-193.4
7 0-16	66.3	-68.8	1 1 -5	25.9	-21.6
7 0-14	68.0	75.5	1 1 -4	18.3	-14.4
7 0-12	56.8	59.5	1 1 -3	57.9	-55.9
7 0-10	31.2	-26.9	1 1 -2	239.4	251.1
7 0 -6	169.6	-163.5	1 1 -1	124.2	118.2
7 0 -4	24.3	15.6	1 1 2	64.3	-63.0
7 0 -2	252.5	234.1	1 1 3	23.0	16.9
7 0 0	69.9	-72.6	1 1 4	93.4	-92.7
7 0 2	61.7	-55.2	1 1 5	88.3	89.1
7 0 6	57.7	-59.4	1 1 6	83.9	-87.2
7 0 8	73.8	83.1	1 1 7	81.1	-83.2
7 0 12	56.8	-57.7	1 1 8	124.5	130.3
8 0-20	49.3	47.1	1 1 9	27.2	24.1
1 1 10	50.6	53.9	5 1 6	45.5	-44.2
1 1 11	30.9	25.6	5 1 8	76.6	-81.2
1 1 12	57.6	-61.4	5 1 9	45.3	-39.1
1 1 13	41.8	-38.7	5 1 11	34.1	32.9
2 1-13	40.4	38.6	6 1-16	30.7	21.4
2 1-11	49.5	-49.7	6 1-15	36.2	-35.8
2 1-10	125.3	131.2	6 1-14	59.2	62.4
2 1 -9	37.9	37.2	6 1-13	43.6	42.3
2 1 -8	36.0	31.0	6 1-12	65.5	-67.0
2 1 -7	71.5	62.7	6 1-10	95.3	-98.0
2 1 -6	180.9	-186.2	6 1 -9	48.7	-49.0
2 1 -5	103.0	-104.1	6 1 -8	65.0	68.1
2 1 -4	18.8	-16.2	6 1 -7	66.5	69.1
2 1 -3	99.9	95.3	6 1 -6	49.3	48.2
2 1 -2	63.5	56.3	6 1 -5	54.7	-53.0
2 1 0	128.6	136.3	6 1 -4	75.6	71.8
2 1 1	83.8	-78.7	6 1 -3	36.8	-32.3
2 1 2	155.4	149.9	6 1 -1	82.9	87.5
2 1 3	106.8	106.5	6 1 0	170.6	-182.7
2 1 4	166.9	-169.0	6 1 1	86.1	-86.3
2 1 5	38.1	-37.2	6 1 2	44.0	34.4
2 1 6	89.6	-88.6	6 1 4	99.0	107.3
2 1 7	39.1	-42.5	6 1 5	44.1	39.4
2 1 8	84.8	94.3	6 1 7	53.0	-56.8
2 1 9	62.0	66.1	6 1 10	37.2	-34.7
2 1 10	28.0	23.4	6 1 14	38.8	39.7
2 1 11	32.1	-32.6	7 1-18	38.7	-36.8
2 1 16	41.4	-39.4	7 1-16	41.8	39.0
3 1-15	45.7	42.1	7 1-14	59.3	65.9
3 1-14	71.3	-77.1	7 1-13	41.8	38.7
3 1-12	29.5	-27.0	7 1-12	43.4	-42.0
3 1-11	41.3	-40.2	7 1-11	45.8	-47.8
3 1-10	114.4	119.3	7 1-10	37.1	-35.2
3 1 -9	73.4	72.9	7 1 -9	34.4	30.5
3 1 -8	23.8	15.6	7 1 -8	42.9	-48.2
3 1 -7	41.5	-38.8	7 1 -7	28.8	26.6
3 1 -6	30.9	-22.4	7 1 -6	25.2	12.8
3 1 -5	19.6	6.7	7 1 -5	83.5	-83.2
3 1 -4	94.8	-92.2	7 1 -4	164.4	173.7
3 1 -3	107.3	107.2	7 1 -3	72.7	72.7
3 1 -2	171.5	-168.6	7 1 -2	40.3	-31.3
3 1 -1	141.2	-132.4	7 1 0	124.3	-122.0
3 1 0	162.5	173.3	7 1 1	62.7	-63.5
3 1 1	36.4	35.4	7 1 3	65.2	60.2
3 1 2	124.5	122.8	7 1 5	37.4	-32.8
3 1 3	78.2	80.4	7 1 6	47.7	49.7
3 1 4	112.8	-116.6	7 1 7	27.4	-20.4
3 1 5	77.8	-79.3	7 1 8	33.9	32.3
3 1 6	37.9	-36.7	7 1 9	33.1	34.9
3 1 7	43.4	41.7	7 1 10	56.0	-59.9
3 1 8	39.4	-34.7	7 1 11	32.6	-29.3
3 1 11	43.8	-41.5	8 1-18	35.8	-39.2
3 1 12	60.8	68.5	8 1-15	29.3	25.3
3 1 13	34.4	34.4	8 1-14	28.0	24.5
4 1-18	45.7	42.7	8 1-13	24.1	-20.1
4 1-15	33.1	27.7	8 1-12	41.5	40.5
4 1-14	67.5	-73.9	8 1 -9	62.7	67.3
4 1-13	42.5	-40.4	8 1 -8	133.8	-144.6
4 1-11	41.5	41.2	8 1 -7	54.9	-57.4
4 1-10	28.9	16.4	8 1 -5	22.1	-18.4
4 1 -9	23.3	20.6	8 1 -4	123.9	127.5
4 1 -8	62.8	65.4	8 1 -3	51.9	49.9
4 1 -7	78.1	-79.6	8 1 -1	66.5	-71.5
4 1 -6	121.0	124.3	8 1 1	36.1	29.3
4 1 -5	103.3	99.1	8 1 2	68.6	-71.8
4 1 -4	160.5	-163.3	8 1 4	62.7	-50.8
4 1 -3	20.8	-11.7	8 1 5	59.0	-60.7
4 1 -2	127.5	-128.9	8 1 6	69.4	82.4
4 1 -1	70.1	-68.0	8 1 7	31.4	30.3
4 1 0	147.1	147.3	8 1 10	34.7	-32.7
4 1 1	90.4	96.2	9 1-16	27.7	-24.2
4 1 2	56.0	55.1	9 1-13	45.6	-43.6
4 1 3	68.3	-66.8	9 1-12	98.7	96.8
4 1 4	54.8	48.5	9 1-11	30.5	28.2
4 1 5	24.9	-19.0	9 1 -8	91.5	-96.6
4 1 6	22.9	-18.9	9 1 -7	51.5	-52.2
4 1 7	55.6	56.7	9 1 -5	60.8	58.7
4 1 8	94.7	-103.7	9 1 -4	23.3	-.2
4 1 9	52.7	-54.1	9 1 -3	39.9	-33.8
4 1 10	45.2	37.6	9 1 -2	71.7	75.7
4 1 12	50.2	50.5	9 1 -1	43.9	-41.8
5 1-18	46.3	41.3	9 1 0	67.9	69.9
5 1-12	43.1	-41.6	9 1 1	57.3	55.7
5 1-11	55.0	57.8	9 1 2	89.1	-96.8
5 1-10	88.6	-94.9	9 1 3	46.3	-43.1
5 1 -9	60.7	-64.7	9 1 4	37.6	-26.5
5 1 -8	115.0	119.2	9 1 6	52.0	42.1
5 1 -7	18.6	16.5	10 1-17	29.1	25.3
5 1 -6	135.5	139.7	10 1-16	53.5	-59.2
5 1 -5	76.6	81.0	10 1-12	57.5	58.6
5 1 -4	110.8	-110.6	10 1-11	37.9	35.4
5 1 -3	94.3	-91.7	10 1 -9	44.4	-44.0
5 1 -2	78.1	-73.3	10 1 -7	21.4	17.3
5 1 -1	58.0	56.4	10 1 -6	62.2	-64.1
5 1 0	71.5	-68.7	10 1 -5	32.8	25.3
5 1 1	28.9	23.4	10 1 -4	70.2	-69.2
5 1 2	34.9	28.3	10 1 -3	74.0	-69.4
5 1 3	74.4	-77.8	10 1 -2	86.6	98.8
5 1 4	143.8	154.6	10 1 -1	41.0	38.3
5 1 5	62.5	68.2	10 1 0	41.5	34.2

Table 2. Continued. Tetraiodoethylene-pyrazine.

10	1	2	48.8	-51.6	2	2	-4	75.5	74.4	6	2	-3	100.9	102.2	12	2-10	28.0	25.6
10	1	3	47.1	-40.4	2	2	-3	82.9	79.8	6	2	-2	53.6	-52.1	12	2	-9	39.1	40.0
10	1	5	34.0	34.3	2	2	-2	126.9	130.9	6	2	-1	35.7	-30.8	12	2	-7	38.9	-36.1
11	1-20		32.6	32.9	2	2	-1	92.5	-94.4	6	2	0	34.8	35.6	12	2	-6	53.5	-57.8
11	1-16		49.6	-40.9	2	2	0	24.5	-22.7	6	2	1	65.9	-64.7	12	2	-2	39.4	35.3
11	1-13		28.4	26.0	2	2	1	88.3	87.7	6	2	2	73.7	70.2	12	2	-1	48.0	-47.9
11	1-11		26.8	-21.5	2	2	2	103.9	-100.5	6	2	3	74.1	79.4	12	2	1	31.4	33.3
11	1-10		47.4	48.7	2	2	3	42.5	39.1	6	2	4	22.4	22.3	13	2-13		31.6	-28.7
11	1	-9	38.8	-36.7	2	2	4	49.8	-42.4	6	2	5	39.3	-37.6	13	2-10		39.9	39.0
11	1	-8	54.6	60.2	2	2	5	100.3	-99.5	6	2	6	55.9	-59.8	13	2	-6	42.3	-35.8
11	1	-7	49.2	51.4	2	2	6	45.5	41.5	6	2	8	34.5	-30.5	13	2	-5	55.2	44.3
11	1	-6	83.7	-90.7	2	2	7	68.7	70.6	6	2	9	42.2	36.7	13	2	-3	33.6	-32.3
11	1	-5	36.5	-31.5	2	2	8	73.8	71.0	6	2	11	37.7	-36.6	13	2	0	27.3	32.3
11	1	-4	50.6	-46.0	2	2	11	38.2	-33.7	7	2-15		44.7	40.7	13	2	1	28.0	28.8
11	1	-2	47.4	50.7	2	2	12	46.3	-45.3	7	2-12		49.8	-55.9	14	2-14		33.3	-32.0
11	1	-1	36.8	31.3	2	2	13	40.3	37.8	7	2-10		29.9	-27.1	14	2-10		31.6	27.4
11	1	1	46.2	-47.9	3	2-16		33.2	-28.4	7	2	-9	53.1	55.0	14	2	-9	43.4	-37.2
11	1	2	39.9	35.0	3	2-13		52.3	-55.6	7	2	-8	66.6	71.0	14	2	-4	33.3	-33.0
11	1	6	52.2	-49.5	3	2-12		45.3	49.4	7	2	-7	66.7	-69.6	14	2	-3	30.4	-30.2
12	1-14		36.6	-31.9	3	2-11		43.6	43.9	7	2	-6	55.7	58.4	14	2	-1	28.1	28.1
12	1-12		46.1	-46.3	3	2-10		38.7	39.4	7	2	-5	30.3	27.1	0	3	2	23.4	23.6
12	1-11		42.1	-38.7	3	2	-8	46.5	-45.0	7	2	-4	30.4	-26.2	0	3	1	33.4	-32.3
12	1-10		60.8	66.1	3	2	-7	59.8	-59.3	7	2	-3	59.8	62.6	0	3	3	48.2	48.7
12	1	-8	47.7	46.1	3	2	-6	98.1	-98.2	7	2	-2	88.3	-85.6	0	3	4	104.7	103.9
12	1	-6	42.6	-39.6	3	2	-5	100.1	99.8	7	2	-1	76.9	-83.6	0	3	5	14.9	-12.3
12	1	-5	48.4	-42.4	3	2	-4	34.0	31.6	7	2	0	55.4	-49.1	0	3	6	58.4	-59.1
12	1	-3	44.7	40.7	3	2	-3	73.1	-70.7	7	2	1	46.6	48.5	0	3	8	64.5	-64.2
12	1	-2	46.4	-41.1	3	2	-2	115.8	117.0	7	2	2	62.5	59.5	0	3	9	20.8	16.2
12	1	2	58.9	63.9	3	2	-1	63.3	-61.9	7	2	4	45.7	41.6	0	3	10	37.0	37.0
12	1	3	39.0	35.1	3	2	0	56.7	52.0	7	2	5	54.4	-50.7	0	3	11	25.5	-23.1
12	1	4	30.0	-27.9	3	2	1	112.4	114.6	7	2	6	26.5	-27.2	1	3-14		24.7	23.8
13	1-16		39.8	32.3	3	2	2	53.3	-49.5	7	2	7	45.2	48.7	1	3-12		42.9	-43.0
13	1-14		45.3	-42.0	3	2	3	80.0	-76.3	7	2	8	33.3	-32.0	1	3-10		45.9	-49.9
13	1-12		41.3	-38.1	3	2	4	94.4	-94.9	8	2-16		32.0	32.7	1	3	-8	75.3	75.9
13	1-10		27.3	25.3	3	2	7	53.0	50.2	8	2-13		33.3	-31.6	1	3	-7	36.3	-36.4
13	1	-9	28.6	25.0	3	2	8	65.0	63.7	8	2-12		46.5	-44.7	1	3	-6	25.4	24.2
13	1	-7	38.1	-35.1	3	2	9	56.2	-57.8	8	2-11		48.9	54.8	1	3	-5	28.9	29.8
13	1	-6	41.6	37.2	3	2	11	25.8	25.6	8	2-10		41.7	-43.4	1	3	-3	40.2	43.1
13	1	-3	30.2	26.2	4	2-17		34.3	32.1	8	2	-8	14.1	14.8	1	3	-2	15.6	-18.6
13	1	-2	61.9	-72.1	4	2-16		32.7	-25.1	8	2	-7	58.6	-61.7	1	3	-1	31.9	-32.1
13	1	-1	45.6	-41.5	4	2-15		26.5	-27.0	8	2	-6	58.8	60.7	1	3	1	24.2	25.2
13	1	2	34.6	28.4	4	2-14		27.4	-24.6	8	2	-5	72.4	76.1	1	3	2	68.2	67.1
14	1-13		31.3	-21.5	4	2-12		36.1	31.5	8	2	-4	37.3	37.5	1	3	4	99.9	96.4
14	1-11		27.4	24.9	4	2-11		44.1	45.3	8	2	-3	35.8	-33.6	1	3	5	22.0	-18.0
14	1-10		31.7	-31.0	4	2-10		84.7	87.2	8	2	-2	68.3	-63.9	1	3	6	45.2	-44.3
14	1	-7	35.4	-31.4	4	2	-9	65.0	-66.2	8	2	-1	26.5	-23.3	1	3	7	37.4	39.6
14	1	-6	73.0	66.9	4	2	-7	49.1	48.5	8	2	0	56.5	-57.9	1	3	10	30.6	-25.7
14	1	-2	33.4	-33.0	4	2	-6	87.9	-89.6	8	2	1	47.4	53.1	1	3	11	22.2	-20.5
15	1-10		52.9	-56.3	4	2	-5	47.0	48.8	8	2	3	60.7	-64.7	1	3	14	44.8	45.0
15	1	-6	41.2	33.2	4	2	-4	55.1	-56.0	8	2	4	42.2	32.1	2	3-14		34.2	33.5
15	1	0	38.9	-31.5	4	2	-3	107.1	-107.4	8	2	7	36.9	34.1	2	3-12		44.1	-48.6
16	1-14		44.3	38.9	4	2	-2	54.3	51.6	8	2	9	33.3	-39.6	2	3-11		35.0	33.4
16	1-10		34.5	-27.9	4	2	-1	98.5	94.8	9	2-16		27.5	29.5	2	3-10		20.9	-19.3
16	1	-4	33.8	30.4	4	2	0	122.6	125.0	9	2-15		30.9	-32.1	2	3	-7	25.3	-22.9
17	1	-4	31.5	33.7	4	2	1	25.1	19.5	9	2-14		33.4	34.6	2	3	-5	38.3	37.2
0	2	0	105.2	-102.5	4	2	3	71.7	-68.3	9	2-11		46.6	46.1	2	3	-4	107.8	109.7
0	2	1	125.5	-118.4	4	2	4	91.9	-92.0	9	2-10		48.1	-54.1	2	3	-3	18.5	-17.8
0	2	2	47.6	-47.5	4	2	5	79.8	79.5	9	2	-9	47.7	-50.1	2	3	-2	52.4	-52.7
0	2	3	20.8	20.8	4	2	6	38.3	-33.0	9	2	-8	40.8	-39.5	2	3	0	104.9	-108.5
0	2	4	86.3	89.6	4	2	7	34.7	-28.4	9	2	-7	32.0	27.5	2	3	1	33.3	33.2
0	2	5	71.8	70.5	4	2	9	24.3	-25.1	9	2	-6	49.6	53.2	2	3	2	49.4	49.5
0	2	6	88.7	88.3	4	2	10	44.0	36.5	9	2	-4	56.7	59.4	2	3	3	42.1	-42.1
0	2	7	81.1	-77.5	4	2	11	50.6	49.0	9	2	-3	59.3	-60.8	2	3	4	20.7	16.0
0	2	8	32.4	-31.7	5	2-15		27.0	-23.6	9	2	-2	32.3	-28.7	2	3	6	40.6	40.2
0	2	9	47.5	46.5	5	2-14		46.7	-43.9	9	2	-1	64.3	70.4	2	3	7	30.9	28.5
0	2	10	48.7	-50.1	5	2-13		41.8	44.7	9	2	0	49.9	-53.2	2	3	8	19.3	18.3
0	2	13	45.8	-43.4	5	2-11		35.9	-33.7	9	2	2	35.6	-31.7	2	3	9	26.0	-24.5
0	2	15	41.9	34.8	5	2-10		59.7	63.4	9	2	3	46.4	-45.8	2	3	10	59.1	-66.9
1	2-14		41.0	35.5	5	2	-9	37.3	-41.4	9	2	5	47.6	45.9	2	3	14	26.9	28.3
1	2-13		33.3	28.6	5	2	-8	41.5	47.4	9	2	6	40.7	35.6	3	3-16		26.3	28.7
1	2-12		34.7	30.7	5	2	-7	97.4	100.6	10	2-15		33.3	-30.1	3	3-11		23.7	22.5
1	2-11		51.3	-54.7	5	2	-6	31.9	-27.2	10	2-14		32.1	29.9	3	3	-9	26.9	-21.6
1	2-10		47.8	-53.8	5	2	-5	54.0	-55.4	10	2-13		36.1	34.2	3	3	-8	82.5	-85.1
1	2	-9	40.7	45.5	5	2	-4	101.2	-102.5	10	2-12		28.0	29.0	3	3	-7	19.2	16.2
1	2	-8	62.4	-68.0	5	2	-3	27.3	-23.4	10	2-10		39.7	-37.4	3	3	-6	43.8	41.0
1	2	-6	44.6	44.7	5	2	-2	26.2	-20.4	10	2	-8	55.8	-61.5	3	3	-4	114.6	110.1
1	2	-5	103.7	-106.8	5	2	-1	69.8	65.9	10	2	-7	47.5	53.4	3	3	-3	26.1	-22.2
1	2	-4	113.7	113.8	5	2	0	86.6	90.5	10	2	-5	53.2	-58.9	3	3	-2	44.3	-44.6
1	2	-3	112.6	113.6	5	2	1	99.3	-89.3	10	2	-4	44.5	43.0	3	3	-1	55.4	54.0
1	2	-2	70.7	74.0	5	2	2	38.3	39.2	10	2	-2	34.9	31.5	3	3	0	19.6	-17.7
1	2	-1	13.2	-9.6	5	2	3	42.0	43.7	10	2	-1	46.1	47.9	3	3	2	43.3	-40.4
1	2	1	91.1	-92.1	5	2	4	34.3	-29.7	10	2	0	29.4	-28.4	3	3	3	40.4	-39.3
1	2	2	108.2	-105.4	5	2	5	45.6	44.8	10	2	1	49.3	-53.4	3	3	4	25.6	-21.3
1	2	3	100.7	96.3	5	2	6	57.1	-58.5	10	2	2	50.2	-55.3	3	3	5	31.3	29.9
1	2	4	55.4	50.3	5	2	7	66.8	-70.3	10	2	7	34.5	-36.5	3	3	6	94.3	96.3
1	2	5	62.7	-60.2	5	2	8	24.4	-22.3	11	2-12		40.8	39.5	3	3	10	41.7	-41.3
1	2	6	90.0	88.4	5	2	9	32.1	31.1	11	2-11		39.7	-40.8	4	3-12		55.6	61.2
1	2	8	33.7	28.6	5	2	10	41.7	35.9	11	2	-9	41.3	44.4	4	3-10		20.4	-18.7
1	2	9	72.6	71.1	6	2-18		30.0	32.4	11	2	-8	46.1	-42.7	4	3	-8	83.7	-86.6
1	2	10	34.6	-32.9	6	2-17		28.6	-28.0	11	2	-6	38.2	-33.6	4	3	-7	32.2	33.8
1	2	11	47.4	-48.7	6	2-14		40.2	-39.9	11	2	-5	48.2	-50.4	4	3	-6	31.1	31.7
1	2	12	44.7	-44.5	6	2-13		36.9	34.1	11	2	-3	44.6	46.7	4	3	-5	45.1	-45.0
2	2-15		34.3	30.9	6	2-12		32.2	-29.4	11	2	-2	51.0	52.0	4	3	-4	24.1	21.7
2	2-14		36.2	31.4	6	2-11		58.2	-60.7	11	2	2	38.5	-33.7	4	3	-2	50.0	51.4
2	2-13		37.9	-30.6	6	2-10		31.0	27.1	11	2	3	44.1	41.7	4	3	-1	44.9	44.9
2	2-12		50.3	53.7	6	2	-9	36.6	36.9	11	2	5	32.9	-31.3	4	3	0	36.5	36.3
2	2	-9	83.5	85.0	6	2	-8	81.0	86.8	12	2-16		33.5	-32.2	4	3	1	24.1	-20.7
2	2	-8	60.9	-63.0	6	2	-6	27.3	20.5	12	2-15		27.7	26.4	4	3	2	114.9	-116.6
2	2	-7	74.4	-75.3	6	2	-5	63.3	-64.6	12	2-13		30.6	-29.0	4	3	3	16.1	12.7
2	2	-6	46.3	-47.4	6	2	-4	96.0	-96.9	12	2-12		31.8	28.8	4	3	6	61.5	63.2

Table 2. Continued. Tetraiodoethylene-pyrazine.

4	3	7	32.2	-28.1	9	3	-6	67.9	70.5	4	4	-2	17.4	16.3	0 5 9 16.8 15.9
4	3	9	22.7	21.5	9	3	-4	51.8	-52.3	4	4	-1	22.0	16.0	1 5 -9 21.1 17.4
4	3	12	26.4	-19.2	9	3	-2	42.6	-44.9	4	4	0	46.8	-49.0	1 5 -8 18.7 -15.3
5	3-16		35.0	-35.5	9	3	0	24.6	23.8	4	4	2	22.9	-17.6	1 5 -7 12.8 -10.0
5	3-12		52.6	60.3	9	3	1	35.7	-33.2	4	4	4	60.1	63.2	1 5 -6 12.8 -10.9
5	3-11		22.2	-23.1	9	3	4	35.7	33.0	5	4-14		38.9	37.8	1 5 -2 8.1 12.2
5	3-10		22.6	-19.0	10	3-10		48.7	-55.1	5	4-10		31.4	-27.5	1 5 -1 11.1 -18.6
5	3 -9		31.1	32.2	10	3 -8		37.7	37.5	5	4 -5		20.3	-14.7	1 5 1 14.6 22.4
5	3 -8		18.1	-13.5	10	3 -6		43.1	43.9	5	4 -4		48.0	51.4	1 5 2 11.5 -10.0
5	3 -6		32.6	-35.4	10	3 -5		22.4	-21.9	5	4 -2		25.1	23.3	1 5 4 23.2 -24.0
5	3 -5		28.6	-28.8	10	3 -3		32.1	29.9	5	4 -1		28.8	19.9	1 5 5 19.6 -18.0
5	3 -4		37.7	-36.9	10	3 0		38.9	-39.2	5	4 0		68.7	-73.9	1 5 7 15.2 12.4
5	3 -3		26.4	24.8	10	3 4		47.8	51.4	5	4 4		19.4	18.3	2 5 -6 13.4 -11.1
5	3 -2		119.5	116.7	11	3-14		38.8	39.2	5	4 8		23.4	21.6	2 5 -5 19.5 20.9
5	3 -1		27.1	-21.9	11	3-12		27.1	-24.5	5	4 10		25.8	-21.6	2 5 -4 19.3 -21.9
5	3 0		23.7	19.8	11	3-10		38.6	-37.8	6	4-14		21.7	20.2	2 5 -3 15.2 -17.9
5	3 2		64.0	-70.1	11	3 -7		30.9	-27.5	6	4 -9		18.3	15.8	2 5 -2 12.7 13.2
5	3 3		33.3	31.7	11	3 -4		45.2	36.7	6	4 -8		38.3	-38.0	2 5 0 19.5 26.9
5	3 5		29.9	-29.2	11	3 0		50.7	-61.6	6	4 -6		27.3	-25.8	2 5 1 19.1 22.6
5	3 6		22.5	-17.8	12	3-14		27.3	27.5	6	4 -5		19.9	-15.3	2 5 3 16.3 -11.5
5	3 8		27.0	26.5	12	3 -8		34.4	-33.4	6	4 -4		61.9	65.2	2 5 4 14.5 -11.8
5	3 10		36.8	37.4	12	3 -4		52.7	57.6	6	4 0		23.2	-19.4	3 5 -9 16.8 -15.4
5	3 12		30.4	-33.0	12	3 0		26.6	-22.1	6	4 4		35.8	-34.6	3 5 -8 23.9 21.0
6	3-16		40.5	-38.7	13	3 -8		46.4	-49.8	6	4 6		23.1	22.3	3 5 -7 19.1 16.7
6	3-10		31.1	30.8	14	3-12		36.1	36.4	6	4 8		27.0	26.6	3 5 -5 10.4 10.4
6	3 -9		30.5	28.8	0	4 2		35.4	42.0	6	4 10		25.2	-24.3	3 5 -4 21.6 -25.5
6	3 -8		35.2	35.3	0	4 3		14.6	12.1	7	4-12		32.1	27.5	3 5 -3 15.6 -18.1
6	3 -7		19.1	-16.2	0	4 4		22.3	-20.2	7	4-10		25.5	20.8	3 5 -1 12.7 12.0
6	3 -6		97.4	-98.2	0	4 6		57.7	-60.7	7	4 -9		18.8	15.1	3 5 0 14.2 16.8
6	3 -4		25.1	-21.5	0	4 7		16.8	-15.0	7	4 -8		51.1	-52.3	3 5 2 17.1 13.7
6	3 -2		84.1	81.8	0	4 8		34.9	36.5	7	4 -4		24.6	18.8	3 5 5 22.6 19.2
6	3 -1		36.6	-33.8	0	4 10		22.4	21.3	7	4 0		33.3	33.5	3 5 6 22.5 -19.4
6	3 1		37.2	34.1	1	4-12		29.5	-25.3	7	4 1		20.2	17.2	4 5 -8 23.1 21.5
6	3 2		28.5	20.2	1	4-10		44.6	46.0	7	4 2		32.7	-27.6	4 5 -7 17.6 15.7
6	3 4		33.5	-31.7	1	4 -8		27.0	23.2	7	4 4		36.3	-37.6	4 5 -4 11.0 -10.7
6	3 5		35.6	-29.2	1	4 -6		30.4	-30.0	7	4 6		30.2	27.4	4 5 -2 12.2 -12.6
6	3 6		47.6	-52.5	1	4 -2		28.3	-36.6	8	4-12		35.8	38.0	4 5 1 23.8 -22.7
6	3 8		43.2	45.6	1	4 2		69.7	78.4	8	4 -8		18.7	-16.7	4 5 2 23.2 25.3
7	3-12		30.8	-27.5	1	4 3		23.9	25.3	8	4 -4		37.3	-37.0	4 5 3 14.4 13.5
7	3-10		69.9	71.8	1	4 4		38.9	-40.3	8	4 -3		18.1	-15.5	4 5 6 17.0 -17.4
7	3 -8		30.9	29.9	1	4 6		30.5	-28.0	8	4 -2		33.7	25.7	5 5 -6 16.9 13.7
7	3 -6		62.5	-65.4	1	4 12		29.8	25.9	8	4 0		40.7	41.5	5 5 -3 22.8 24.1
7	3 -5		36.4	40.9	2	4-14		30.5	-27.5	8	4 2		37.2	-36.5	5 5 -2 23.9 -23.0
7	3 -3		34.8	-32.3	2	4-10		27.8	25.0	9	4 -8		30.2	30.6	5 5 2 22.6 21.2
7	3 -2		30.6	-23.2	2	4 -6		39.2	39.0	9	4 -6		26.0	-21.7	6 5 -7 21.8 -20.9
7	3 -1		30.8	-27.0	2	4 -4		17.2	-14.5	9	4 -4		41.5	-46.4	6 5 -6 25.2 24.1
7	3 0		36.8	35.9	2	4 -3		15.1	14.5	9	4 -2		29.9	28.9	6 5 -4 12.0 10.8
7	3 1		23.3	20.5	2	4 -2		63.5	-78.7	9	4 6		32.9	-28.5	6 5 -3 12.2 10.8
7	3 2		70.4	70.6	2	4 -1		19.3	-21.0	10	4-12		26.7	-23.0	6 5 -2 20.7 -19.4
7	3 4		50.3	-55.9	2	4 0		38.1	43.7	10	4 -8		35.4	36.2	7 5 -6 18.8 18.1
7	3 6		27.3	-25.6	2	4 2		39.4	41.6	10	4 -6		30.5	-28.0	7 5 -4 13.1 10.4
8	3-14		42.6	-43.5	2	4 6		15.8	10.8	10	4 2		34.1	29.4	7 5 -3 13.8 -11.1
8	3-12		23.4	-21.0	2	4 8		38.1	-37.4	10	4 6		27.3	-27.5	8 5 -4 14.4 9.5
8	3-10		48.3	51.4	2	4 12		38.4	34.8	11	4-12		31.8	-31.1	8 5 -3 15.9 -13.9
8	3 -9		33.4	-32.9	3	4-10		27.3	-25.7	11	4 -2		36.1	-35.2	9 5 -6 16.5 -14.9
8	3 -6		24.6	21.8	3	4 -6		66.8	72.3	11	4 2		32.5	30.9	9 5 -5 19.2 -17.2
8	3 -4		30.2	-27.4	3	4 -5		21.5	17.7	12	4 -6		31.8	29.6	10 5 -6 16.3 -16.7
8	3 -3		30.3	-22.4	3	4 -4		30.1	-30.3	12	4 -2		34.4	-34.4	0 6 0 7.7 -12.4
8	3 -2		75.3	-74.5	3	4 -2		35.6	-37.3	13	4-10		24.4	-26.4	1 6 -4 14.9 13.8
8	3 -1		21.7	19.3	3	4 2		18.0	-15.3	13	4 -6		34.1	28.7	1 6 -3 7.7 -7.0
8	3 0		55.6	57.4	3	4 4		47.6	47.7	14	4-10		25.7	-24.8	1 6 3 12.9 -11.1
8	3 2		38.0	35.6	3	4 5		17.2	14.4	0	5 2		12.0	-14.5	2 6 -8 13.0 -10.2
8	3 4		30.6	-23.8	3	4 6		19.8	13.8	0	5 3		16.5	18.2	2 6 -4 9.7 9.2
9	3-14		33.3	-31.1	3	4 8		47.9	-51.4	0	5 4		20.2	-21.0	2 6 -1 11.0 12.3
9	3-13		24.8	23.3	4	4-10		50.2	-49.7	0	5 5		20.4	-19.2	2 6 2 11.5 -10.3
9	3 -9		13.1	-15.7	4	4 -8		27.6	26.9	0	5 6		15.3	13.2	3 6 -2 10.1 10.2
9	3 -8		24.6	23.0	4	4 -6		36.7	37.7	0	5 8		24.9	22.0	4 6 -2 11.8 9.9
															6 6 -5 11.7 10.9

Unobserved reflexions.

0	0	2	3.5	-8.2	9	0	8	23.1	-3.1	15	0-10		16.2	-16.5	5 1-15 13.1 -10.4
1	0	12	14.3	12.0	10	0-12		13.5	13.0	15	0 -6		19.5	28.8	5 1-14 12.4 -4.2
1	0	14	16.0	-23.0	10	0 -8		12.1	14.1	15	0 -4		16.5	2.0	5 1-13 11.8 -3.2
2	0-14		19.7	10.8	10	0 2		14.3	-3.1	15	0 -2		16.5	13.9	5 1 7 11.5 -11.9
2	0	12	14.8	-9.9	10	0 4		16.1	-3.6	16	0 -6		18.1	-15.7	5 1 10 13.4 15.8
3	0	8	12.3	2.9	10	0 6		18.5	2.5	0	1 7		8.7	5.8	6 1-11 10.6 6.6
4	0-14		14.3	11.6	11	0-12		13.9	-18.3	1	1-11		11.1	2.7	6 1 -2 8.5 -7.7
4	0-10		11.3	9.7	11	0 -2		13.9	-16.7	1	1 -8		12.0	8.9	6 1 3 11.2 -6.3
5	0-14		14.1	9.4	11	0 0		14.0	-11.7	1	1 14		14.0	-9.8	6 1 6 11.8 -14.8
5	0 10		15.3	-27.1	11	0 2		15.0	-10.4	2	1-15		13.7	-3.6	6 1 8 13.0 .2
6	0	8	14.7	-4.8	12	0 -6		14.2	7.5	2	1-14		12.9	-18.6	6 1 9 13.6 20.2
7	0	-8	10.6	16.8	12	0 -4		18.2	-.8	2	1-12		12.9	-13.2	7 1-15 13.0 2.2
7	0	4	14.9	-7.3	12	0 -2		14.5	9.0	2	1 12		13.0	19.3	7 1 -1 10.3 -.8
7	0	10	17.5	19.8	13	0-10		14.5	-22.9	2	1 13		13.8	-5.8	7 1 2 12.3 20.2
8	0-14		14.2	10.6	13	0 -8		14.5	-6.1	3	1-13		12.0	-4.6	7 1 4 13.1 3.8
8	0-12		13.0	-12.6	13	0 -6		16.2	-4.6	3	1 9		11.5	-.4	8 1-16 13.6 21.1
8	0 -8		11.0	3.5	14	0-12		15.6	3.6	3	1 10		12.2	16.5	8 1-11 10.9 -17.8
8	0 0		11.9	4.3	14	0-10		15.3	3.6	4	1-16		13.9	18.1	8 1-10 10.4 -2.8
9	0-12		13.2	-13.7	14	0 -6		21.2	21.1	4	1-12		11.2	-13.6	8 1 -6 12.2 12.8
9	0 -4		11.8	-13.6	14	0 -2		15.8	-31.3	4	1 11		13.4	4.8	8 1 -2 14.7 -6.5
9	0	6	21.8	7.2	14	0	0	16.3	3.4	5	1-16		13.7	13.2	8 1 0 13.8 -9.8

Table 2. Continued. Tetraiodoethylene-pyrazine.

8	1 3	13.7	18.7	6	2 7	11.8	-9.6	4	3-11	9.4	-5.2	1	4 -9	8.9	-1.5
8	1 8	15.9	15.8	7	2-14	11.7	-5.9	4	3 -9	8.3	12.5	1	4 -7	7.6	13.4
9	1-15	13.1	17.9	7	2-13	11.2	-20.4	4	3 -3	5.6	-1.2	1	4 -5	6.3	-2.7
9	1-14	12.6	-2.4	7	2-11	10.2	-10.0	4	3 4	8.0	-5.6	1	4 -4	5.6	2.0
9	1-10	10.7	1.5	7	2 3	14.4	20.2	4	3 5	8.5	3.4	1	4 -3	4.7	5.0
9	1 -9	13.8	4.8	8	2-15	12.4	6.8	4	3 8	10.2	-4.4	1	4 -1	7.2	-12.7
9	1 -6	9.9	-3.5	8	2-14	11.8	18.5	5	3-13	10.4	-2.0	1	4 1	4.0	-3.6
9	1 5	16.5	-8.2	8	2 -9	9.5	-17.5	5	3 -7	7.4	5.7	1	4 5	7.0	-3.6
9	1 7	20.7	26.0	8	2 -8	9.2	14.8	5	3 1	9.7	-15.2	1	4 7	8.3	-3.7
10	1-15	13.3	-22.3	8	2 2	11.2	19.8	5	3 4	8.9	6.1	1	4 8	9.0	10.8
10	1-14	12.8	-4.5	8	2 5	15.6	7.3	5	3 7	10.3	-12.4	1	4 9	9.6	1.3
10	1-13	12.3	-12.6	8	2 6	14.9	18.6	5	3 9	11.4	16.4	2	4 -9	8.7	-.9
10	1-10	11.1	7.7	8	2 8	15.2	-20.4	6	3-13	10.4	-19.7	2	4 -8	8.1	3.3
10	1 -8	10.7	1.2	9	2-13	11.5	6.7	6	3-12	9.9	14.6	2	4 -7	7.5	-8.6
10	1 1	12.1	9.7	9	2-12	11.0	-11.5	6	3-11	9.4	-.6	2	4 -5	6.2	10.2
10	1 4	14.1	-7.9	9	2 -5	10.6	16.8	6	3 -5	7.1	13.3	2	4 1	5.2	-1.8
10	1 6	16.2	-29.1	9	2 1	10.9	.2	6	3 -3	7.0	7.6	2	4 3	6.3	3.4
11	1-15	13.5	-20.4	9	2 4	13.6	22.1	6	3 0	8.2	.4	2	4 4	6.9	-8.3
11	1-14	13.0	-9.5	10	2-11	10.9	-15.2	6	3 3	10.2	11.5	2	4 5	7.6	1.7
11	1-12	12.2	-3.9	10	2 -9	10.3	-14.6	6	3 7	11.0	14.1	2	4 7	8.8	12.3
11	1 -3	13.4	-18.8	10	2 -6	10.0	6.1	7	3-13	10.5	-13.3	3	4 -9	8.6	-4.0
11	1 0	12.3	12.8	10	2 -3	15.1	-4.2	7	3-11	9.5	8.3	3	4 -8	8.0	11.5
11	1 3	13.7	11.2	10	2 3	12.6	17.3	7	3 -9	8.6	-16.4	3	4 -7	7.4	-12.5
11	1 4	14.3	-16.4	10	2 4	13.3	5.9	7	3 -7	8.0	-3.6	3	4 -3	5.2	5.2
11	1 5	15.1	20.0	10	2 5	14.2	13.1	7	3 -4	7.6	-5.7	3	4 -1	5.3	.7
12	1-15	13.8	3.1	11	2-14	12.4	20.9	7	3 3	13.9	-19.7	3	4 0	6.8	9.0
12	1-13	13.0	19.6	11	2-13	11.9	8.6	7	3 5	11.6	3.2	3	4 1	6.6	6.5
12	1 -9	12.0	18.3	11	2-10	11.0	-9.8	7	3 7	12.1	6.3	3	4 3	7.0	-10.3
12	1 -7	12.1	8.0	11	2 -7	10.7	5.6	8	3-13	10.6	12.5	3	4 7	9.3	8.8
12	1 -4	15.9	-16.1	11	2 -4	14.4	19.8	8	3-11	9.7	6.5	4	4 -9	8.6	-10.4
12	1 -1	12.8	-9.0	11	2 -1	11.5	-18.1	8	3 -8	8.6	8.5	4	4 -7	7.4	-5.7
12	1 0	13.0	16.9	11	2 0	11.7	-7.8	8	3 -7	8.4	15.5	4	4 -5	6.4	3.4
12	1 1	13.3	-26.7	11	2 1	12.0	-19.1	8	3 -5	8.2	13.8	4	4 -4	6.0	-6.7
13	1-13	13.4	-13.8	11	2 4	13.6	-10.2	8	3 1	9.7	-11.7	4	4 -3	5.8	-.2
13	1-11	12.9	-16.9	12	2-14	12.7	-2.3	8	3 3	11.9	-19.7	4	4 1	9.0	-12.1
13	1 -8	12.7	12.9	12	2-11	11.7	-8.0	8	3 5	15.0	24.4	4	4 3	7.9	-11.9
13	1 -5	19.3	7.2	12	2 -8	11.4	-21.0	8	3 6	14.3	4.4	4	4 5	8.8	13.6
13	1 -4	14.2	-15.7	12	2 -5	13.6	14.7	9	3-12	10.3	-8.8	4	4 6	9.3	-5.5
13	1 0	13.6	24.1	12	2 -4	14.9	-3.1	9	3-11	9.9	-14.2	5	4 -9	8.6	1.0
13	1 1	14.0	15.7	12	2 -3	12.4	17.8	9	3-10	9.6	-15.9	5	4 -8	8.1	4.5
14	1-14	14.2	-16.0	12	2 0	12.3	12.5	9	3 -9	9.3	-15.7	5	4 -7	7.6	3.5
14	1-12	13.6	-11.7	12	2 2	13.0	-9.1	9	3 -7	8.9	17.4	5	4 -6	7.2	-11.5
14	1 -9	13.5	-5.7	13	2-12	12.4	6.7	9	3 -5	8.9	-17.0	5	4 -3	6.5	8.8
14	1 -8	13.8	11.4	13	2-11	12.2	22.0	9	3 -3	11.1	6.1	5	4 1	9.9	-7.5
14	1 -5	15.6	31.7	13	2 -9	12.0	-13.6	9	3 -1	9.8	12.8	5	4 2	9.3	-1.2
14	1 -4	14.2	-20.9	13	2 -8	12.1	3.1	9	3 2	10.7	-5.1	5	4 3	9.0	3.7
14	1 -3	13.9	-12.6	13	2 -7	12.5	-18.7	9	3 3	11.5	7.9	5	4 5	9.6	-3.1
14	1 -1	14.0	-8.7	13	2 -4	13.5	-19.8	10	3-12	10.5	-12.0	5	4 6	10.0	-2.2
14	1 0	14.3	7.7	13	2 -2	12.6	5.5	10	3-11	10.2	-10.2	6	4-10	9.2	13.9
15	1-12	14.3	-7.6	13	2 -1	12.7	-15.0	10	3 -9	9.7	9.0	6	4 -7	7.9	.6
15	1-11	14.2	19.5	14	2-12	13.0	-7.6	10	3 -7	9.4	-16.9	6	4 -3	7.3	8.2
15	1 -9	14.5	-26.5	14	2-11	12.8	14.2	10	3 -4	10.6	-20.6	6	4 -2	7.9	5.0
15	1 -8	15.3	12.7	14	2 -8	13.1	17.4	10	3 -2	10.6	2.2	6	4 -1	10.0	.1
15	1 -7	18.9	10.8	14	2 -7	14.0	23.1	10	3 -1	10.3	-9.3	6	4 1	9.4	6.2
15	1 -5	15.0	11.5	14	2 -6	18.4	-7.1	10	3 1	10.7	-21.2	6	4 2	12.9	-2.1
15	1 -4	14.5	-3.6	14	2 -5	14.7	13.6	10	3 2	11.2	-4.2	6	4 3	10.7	6.3
15	1 -3	14.4	-25.6	14	2 -2	13.1	-13.6	10	3 3	11.7	10.9	7	4 -7	8.2	-1.7
15	1 -2	14.5	4.8	15	2 -9	13.8	-15.2	11	3-11	10.6	7.6	7	4 -6	8.0	-5.5
16	1 -9	16.1	-9.7	15	2 -8	14.7	27.2	11	3 -9	10.1	15.2	7	4 -5	7.8	.7
16	1 -8	19.0	-1.7	15	2 -7	18.4	25.4	11	3 -8	10.0	14.5	7	4 -3	8.2	-5.1
16	1 -7	18.5	21.2	15	2 -6	16.0	14.9	11	3 -6	10.2	-.8	7	4 -2	10.0	-1.2
16	1 -6	15.9	-7.0	15	2 -5	14.2	-23.7	11	3 -5	10.8	.7	7	4 -1	9.4	-7.7
0	2 11	10.9	8.6	0	3 7	7.7	-3.7	11	3 -3	11.8	12.9	7	4 3	14.4	-4.0
0	2 12	11.5	-14.6	0	3 12	10.8	6.5	11	3 -2	10.8	5.4	8	4 -9	9.2	2.8
1	2 13	12.6	1.1	1	3-11	9.9	8.3	11	3 -1	10.8	-14.5	8	4 -7	8.6	6.9
2	2-11	10.3	-13.3	1	3 -9	8.7	15.2	11	3 1	11.2	14.7	8	4 -6	8.5	-5.6
1	2 -7	7.9	13.5	1	3 -4	5.4	2.0	12	3-11	11.0	18.1	8	4 -5	8.4	10.2
1	2 7	8.6	-17.1	1	3 3	5.4	7.0	12	3-10	10.8	-1.1	8	4 -1	9.6	1.2
2	2-10	9.7	-11.5	1	3 8	8.7	-10.0	12	3 -9	10.7	-2.7	8	4 1	10.0	11.4
2	2 -5	6.4	-4.8	1	3 9	9.3	-6.9	12	3 -7	10.8	-15.7	9	4 -9	9.5	-9.2
2	2 9	10.4	6.9	2	3-13	10.9	-7.9	12	3 -6	11.2	-11.4	9	4 -7	9.1	14.1
2	2 10	11.0	-9.9	2	3 -9	8.5	-10.1	12	3 -5	13.1	8.2	9	4 -5	9.2	4.8
3	2-15	12.7	13.0	2	3 -8	7.9	-2.3	12	3 -3	11.6	-17.2	9	4 -3	11.8	-10.9
3	2-14	12.0	14.9	2	3 -6	6.6	9.6	12	3 -2	11.3	-6.9	9	4 -1	10.0	.4
3	2 -9	8.9	2.4	2	3 -1	3.9	.7	12	3 -1	11.3	-2.6	9	4 0	10.1	10.5
3	2 5	8.4	-5.7	2	3 5	7.3	7.7	13	3 -9	11.3	-8.6	10	4 -7	9.7	6.9
3	2 6	9.0	7.4	2	3 11	11.0	3.2	13	3 -7	11.7	12.4	10	4 -5	10.0	-.9
3	2 10	11.5	12.7	3	3-13	10.7	11.3	13	3 -6	13.1	1.3	10	4 -4	11.1	-14.8
3	2 12	12.8	-16.8	3	3-12	10.1	.2	13	3 -5	16.2	-2.0	10	4 -3	13.9	8.7
4	2-13	11.2	-4.1	3	3-10	8.9	-5.1	13	3 -4	12.5	21.7	10	4 -2	10.8	-2.3
4	2 -8	8.2	2.9	3	3 -5	6.0	2.5	13	3 -3	11.9	-20.2	0	5 1	5.2	-.9
4	2 2	7.9	7.6	3	3 1	6.3	-7.1	0	4 0	6.9	2.4	1	5 -3	3.7	4.6
4	2 8	10.8	20.3	3	3 7	9.0	-6.2	0	4 1	6.9	-6.5	2	5 -1	3.2	-4.1
5	2-12	10.6	-.1	3	3 8	9.6	-1.9	0	4 5	6.6	3.2	3	5 -2	3.9	5.9
6	2-15	12.3	17.4	3	3 9	10.2	-7.3	0	4 9	9.2	9.0				
6	2 -7	8.1	10.4	4	3-13	10.5	15.4								

statistical criteria regarding such F_o values are valid.[5] The F_o values adopted were obtained by putting I equal to $\frac{1}{4} I_{min}$ and given a weight equal to $\frac{1}{3} A1$. In the case of the tetraiodoethylene adduct scale factors were recalculated before starting the two last refinement cycles and in such a way that for each layer $\sum|F_o|$ equals $\sum|F_c|$.

Table 3. Atomic coordinates and thermal parameters according to the expression $\exp-(B_{11}h^2+B_{22}k^2+B_{33}l^2+B_{12}hk+B_{13}hl+B_{23}kl)$.

(Estimated standard deviations in parantheses).

Tetrabromoethylene

Molecule No. 1	x	y	z
X1	.1518	.1120	.1509
	(.0004)	(.0016)	(.0004)
X2	−.0888	.1984	.1076
	(.0004)	(.0014)	(.0004)
C1	.054	−.007	.023
	(.003)	(.013)	(.004)
Molecule No. 2			
X1	.5883	.2842	.1838
	(.0004)	(.0013)	(.0004)
X2	.3474	.3756	.0138
	(.0003)	(.0015)	(.0004)
C1	.534	.474	.021
	(.003)	(.012)	(.004)

Molecule No. 1	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
X1	.0069	.126	.0087	−.008	.0017	−.002
	(.0004)	(.005)	(.0005)	(.003)	(.0006)	(.003)
X2	.0102	.105	.0096	.012	.0118	.003
	(.0004)	(.005)	(.0005)	(.002)	(.0007)	(.003)
Molecule No. 2						
X1	.0089	.097	.0082	.005	.0054	.007
	(.0004)	(.005)	(.0004)	(.002)	(.0006)	(.002)
X2	.0062	.114	.0132	−.008	.0102	−.004
	(.0003)	(.005)	(.0005)	(.002)	(.0007)	(.003)

Isotropic thermal parameters for the C-atoms:
Molecule No. 1: 6.6 (1.3) Molecule No. 2: 4.7 (1.0)

Tetrabromoethylene-pyrazine	x	y	z
X1	.19411	.0233	.15267
	(.00015)	(.0005)	(.00013)
X2	−.09274	.2411	.11376
	(.00015)	(.0005)	(.00013)
N1	.4235	.078	.3803
	(.0015)	(.005)	(.0014)
C1	.0554	−.041	.0084
	(.0014)	(.004)	(.0013)
C3	.5276	−.096	.4086
	(.0020)	(.005)	(.0018)
C6	.3953	.167	.4715
	(.0018)	(.005)	(.0020)

Table 3. Continued.

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
X1	.00637 (.00014)	.0692 (.0013)	.00519 (.00013)	−.0062 (.0008)	.0029 (.0003)	.0030 (.0008)
X2	.00911 (.00013)	.0614 (.0011)	.00606 (.00012)	.0050 (.0009)	.0079 (.0003)	−.0046 (.0008)
N1	.0094 (.0016)	.084 (.014)	.0077 (.0014)	−.003 (.008)	.003 (.002)	−.006 (.007)
C1	.0068 (.0013)	.043 (.010)	.0041 (.0009)	−.002 (.007)	.004 (.002)	.002 (.006)
C3	.010 (.002)	.068 (.014)	.010 (.002)	−.011 (.010)	.007 (.003)	−.006 (.009)
C6	.006 (.002)	.069 (.014)	.013 (.002)	−.001 (.008)	.007 (.003)	.008 (.009)

Tetraiodoethylene-pyrazine	x	y	z
X1	.20406 (.00010)	.1139 (.0003)	.17839 (.00009)
X2	−.11423 (.00011)	.2407 (.0004)	.09990 (.00009)
N1	.412 (.002)	.345 (.006)	.399 (.003)
C1	.0560 (.0014)	−.024 (.004)	.0170 (.0011)
C3	.490 (.002)	.533 (.007)	.394 (.002)
C6	.415 (.002)	.330 (.007)	.501 (.002)

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
X1	.00412 (.00009)	.0613 (.0008)	.00311 (.00007)	−.0069 (.0005)	.00167 (.00011)	−.0043 (.0004)
X2	.00567 (.00010)	.0598 (.0008)	.00377 (.00007)	.0036 (.0005)	.00430 (.00014)	−.0029 (.0004)
N1	.009 (.002)	.065 (.015)	.015 (.003)	−.014 (.009)	.008 (.004)	−.013 (.011)
C1	.0036 (.0011)	.043 (.009)	.0015 (.0008)	−.006 (.006)	.0005 (.0015)	.001 (.005)
C3	.009 (.002)	.10 (.02)	.0032 (.0012)	.011 (.011)	.007 (.003)	−.006 (.008)
C6	.004 (.002)	.08 (.02)	.009 (.002)	−.017 (.009)	.001 (.003)	−.018 (.010)

Table 4. Uncorrected interatomic distances (Å) and angles (°). (See Fig. 1). (Estimated standard deviations in parantheses).

	Tetrabromoethylene Molecule No. 1	Tetrabromoethylene Molecule No. 2	Tetrabromo-ethylene-pyrazine	Tetraiodo-ethylene-pyrazine
X1–X2	3.270 (.005)	3.286 (.006)	3.355 (.002)	3.632 (.001)
X1–X4	3.197 (.007)	3.196 (.006)	3.163 (.002)	3.545 (.002)
X1–X3	4.584 (.008)	4.588 (.009)	4.626 (.003)	5.084 (.002)
X2–X4	4.562 (.009)	4.581 (.006)	4.595 (.003)	5.066 (.002)
C1–C2	1.41 (.09)	1.26 (.08)	1.29 (.03)	1.27 (.03)
X1–N1			3.019 (.015)	2.979 (.026)
N1–N2			2.82 (.03)	2.83 (.05)
N1–C3			1.35 (.02)	1.30 (.03)
N1–C6			1.32 (.02)	1.28 (.04)
C3–C4			1.41 (.03)	1.45 (.03)
∠X1–X2–X3	90.3 (.2)	90.1 (.2)	90.40 (.07)	9.20 (.05)
∠X1–N1–N2			154.6 (.7)	170.1 (1.1)

The number of independent reflexions for the structure determinations were:

	Observed	Not observed
Tetrabromoethylene	328	220
Tetrabromoethylene-pyrazine	606	330
Tetraiodoethylene-pyrazine	1068	426

In Table 2 observed and calculated structure factors are listed, in Tables 3 and 4 the final coordinate values and the interatomic distances and angles directly derived from these coordinates. The pyrazine molecule comes out planar in both addition compounds and the nitrogen-halogen bonds are situated in or at least very near the plane perpendicular to the pyrazine ring and containing its two nitrogen atoms.

In Table 5 corrected values of interatomic distances and angles are listed. An accurate determination of the carbon coordinates of the tetrahalogenoethylene molecules is difficult to achieve. The distance between these atoms was put equal to 1.34 Å and it was assumed that the two non-equivalent carbon-halogen distances were of equal lengths. Slight adjustments of the distances within the pyrazine molecule were performed resulting in complete agreement with the model obtained by Wheatley,[6] and its orientation in space so adjusted that optimal agreement with coordinates resulting from the least-squares refinement is achieved. Interatomic distances within the tetrahalogenoethylene molecule were corrected for rigid-body movements. The number of independent atoms beeing small and the damping factors of carbon atoms not very accurate, an approximate method was chosen, similar to that used by Weathley for pyrazine.[6] An orthogonal coordinate system with origo in the symmetry centre of the molecule was chosen with the z axis perpendicular to the molecular plane, the x and y axes both nearly passing through a pair of equivalent halogen atoms. It was further assumed that the chief axes of the libration ellipsoid coincide with these axes. In this case the corrections (Δr) are expressed by:[7]

$$\Delta r = \frac{1}{2r}\left(\frac{s^2}{(1+(s^2/q^2)} + \frac{t^2}{1+(t^2/q^2)}\right)$$

In this expression r is the distance from the centre of symmetry.

From the B_{ij} values of the halogen atoms the libration about the z axis could be computed, but not the librations about the other axes. For the addition compounds the relevant informations could be obtained by considering the B_{ij} values of the carbon atoms, however. In the case of tetrabromoethylene,

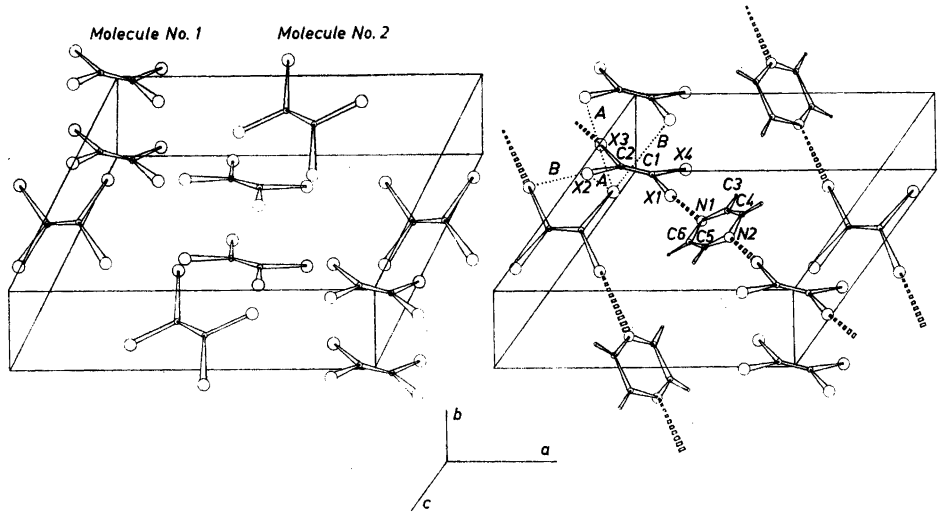

Fig. 1. Structures of tetraiodoethylene [3] and its pyrazine adduct. The designations correspond also to those of the bromine compounds.

Table 5. Corrected interatomic distances (Å) and angles (°). (See Fig. 1).

	Tetrabromoethylene Molecule No. 1	Tetrabromoethylene Molecule No. 2	Tetrabromo-ethylene-pyrazine	Tetraiodo-ethylene-pyrazine
X1—X2	3.289	3.305	3.365	3.638
X1—X4	3.216	3.214	3.172	3.551
X1—X3	4.613	4.613	4.638	5.093
X2—X4	4.588	4.608	4.610	5.074
C1—X1	1.881	1.883	1.881	2.114
X1—N1			3.018	2.979
∠X1—X2—X3	90.3	90.1	90.34	90.21
∠X1—C1—X4	117.6	117.1	115.0	114.2
∠C1—X1—N1			174.8	175.2
∠X1—N1—N2			154.6	172.7

for which the damping parameters of the carbon atoms were not judged to be sufficiently accurate, it was assumed that the $\bar{u}^2$ values of the halogen atoms in the z direction were equally influenced by translation and by libration. The q^2 value in the expression for Δr was put equal to 0.1 Å^2 in all cases.

DISCUSSION

From the figures given in Tables 4 and 5 (*cf.* Fig. 1) it is seen that the parallelogram formed by the four halogen atoms is almost rectangular in solid tetrabromoethylene. In the two addition compounds, however, the diagonal drawn between halogen atoms linked to nitrogen is significantly longer than that drawn between halogen atoms which are not bonded to nitrogen. Apart from this, the structure of the two kinds of acceptor molecules are in close agreement with those derived from electron diffraction measurements in their vapour.[8,9] In the case of tetrabromoethylene a certain difference is found between the structure derived for the gaseous state and the crystals, apparently due to a slight change in the Br—C—Br angle. The C—Hal···N arrangement is very nearly linear in both addition compounds, but the direction of the N—Hal bond does not coincide with that of the line drawn between the nitrogen atoms of the pyrazine molecule. The nitrogen-iodine bond length is found to be slightly shorter than the corresponding separation of nitrogen and bromine (X1—N1, Table 5), and an estimate of the accuracy of the two values confirms the validity of this conclusion.

The mutual arrangements of acceptor molecules within the set of equivalent partners present both in the tetrahalogenoethylene crystals and in the adduct crystals turn out to be virtually identical with closest halogen-halogen contact distances ranging from 3.67 to 4.01 Å in the case of bromine, and from 3.80 to 4.20 Å in the case of iodine. One halogen atom has two close contacts of identical lengths (type A) and a third somewhat closer contact (B). The other halogen atom, in the addition compound linked to nitrogen, exhibits a contact of type B. The A and B contact distances are (in Å):

	C_2Br_4	C_2Br_4-pyrazine	C_2I_4	C_2I_4-pyrazine
A	4.01	3.78	4.20	4.18
B	3.78	3.67	3.80	3.85

It may be noted that a splitting of the adduct crystals parallel to (100) does not involve the breaking of short halogen contacts, although charge-transfer bonds will necessarily be broken. The fact that the (100) face is preferentially being developed in the adduct crystals again points to the relative importance of van der Waals' forces in determining the crystal structure of the addition compounds in question.

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Received March 30, 1968.