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The Structure of the Catecholamines.
III. Crystal Structure of Adrenalone Hydrochloride Monohydrate

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The crystals of adrenalone hydrochloride monohydrate, $C_9H_{11}O_3N\cdot HCl\cdot H_2O$, are monoclinic, space group $P2_1/c$, four formula units in a cell with $a=7\cdot13$, $b=10\cdot14$, $c=17\cdot61$ Å, $\beta=119\cdot0°$. The structure was determined by minimum functions and Fourier synthesis and was refined by least-squares methods to a final R value of 0·048 with 2271 observed reflexions. Estimated standard deviations for bond lengths and angles involving non-hydrogen atoms are in the range of 0·003–0·004 Å and around 0·2°, respectively. The molecule is approximately planar, and the structure is held together by six hydrogen bonds involving all hydrogen atoms on the nitrogen and oxygen atoms.

Introduction

Adrenalone is a catecholamine, structurally resembling the biologically important hormone adrenaline (epinephrine); a carbonyl radical has replaced the alcoholic hydroxyl group on the β-carbon atom. The physiological effect of adrenalone is that of a sympathomimetic amine (Loewi & Meyer, 1905). Despite its resemblance to adrenaline, its action is more like that of noradrenaline. This could be explained by the probable indirect action of adrenalone with an activity about $\frac{1}{10}$ that of noradrenaline (Wennmalm, 1970). It was considered valuable to determine the structure of adrenalone in order to compare it with other catecholamines and related phenethylamines in our research programme.

Experimental

Well developed, water-clear crystals of suitable size were obtained by slow evaporation of an aqueous solution of pure adrenalone hydrochloride (Fluka, Switzerland). The monoclinic crystals were six-sided prisms bounded by {011} (predominant) and {001}, and terminated by {100} (predominant) and $\{10\bar{2}\}$. Twinning was frequently observed; composition plane (010) and twinning axis $= a$. According to Faber (1929), adrenalone hydrochloride monohydrate is dimorphous and crystallizes in an orthorhombic and a monoclinic form, the latter being the stable one at room temperature. Optical properties were also investigated by Faber. In a detailed re-investigation Faber (1930) found that the principal refractive indices differed from crystal to crystal, and he concluded that these differences were caused by crystal imperfections. The crystals are highly birefringent ($\gamma_D-\alpha_D=0\cdot242$).

A suitable crystal was trimmed to an almost spherical shape ($0\cdot42\times0\cdot45\times0\cdot46$ mm). The calculated value of the linear absorption coefficient for Mo $K\alpha$ equals $3\cdot39$ cm^{-1} which is low enough for absorption corrections to be neglected. Unit-cell dimensions were determined in a linear diffractometer. Density was measured by flotation in an xylene-chloroform mixture.

Table 1. *Observed and calculated structure factors*

Items in order are h, k, l, F_o and F_c. Unobserved reflexions are marked with asterisks.

0	0	2	7.5	-12.5
0	0	4	96.6	-101.5
0	0	6	63.8	65.2
0	0	8	19.0	-18.0
0	0	10	20.5	-19.3
0	0	12	56.5	55.7
0	0	14*	0.9	1.8
0	0	16	2.0	-1.8
0	0	18	2.1	2.1
0	0	20	4.7	-4.9
0	1	2	13.5	-12.2
0	1	3	51.5	53.8
0	1	4	23.7	23.2
0	1	5	12.4	-12.9
0	1	6	38.0	-37.1
0	1	7	26.0	-24.2
0	1	8	16.5	-14.7
0	1	9	22.7	21.1
0	1	10	19.6	19.3
0	1	11	1.9	0.2
0	1	12	1.7	1.1
0	1	13	13.1	-13.5
0	1	14	7.4	-7.3
0	1	15	24.7	23.7
0	1	16	2.4	0.1
0	1	17	1.7	-1.6
0	1	18	1.9	-1.3
0	1	19	11.4	-10.8
0	1	20*	1.1	-1.5
0	2	2	45.6	-48.8
0	2	3	3.7	2.7
0	2	4	26.4	-24.9
0	2	5	35.7	34.4
0	2	6	45.3	45.2
0	2	7	45.7	-41.5
0	2	8	27.7	-25.7
0	2	9	6.2	5.4
0	2	10	23.7	-22.2
0	2	11	5.0	-4.8
0	2	12	21.7	21.0
0	2	13	5.2	5.2
0	2	14	12.1	-12.5
0	2	15	5.7	5.4
0	2	16	5.5	-5.9
0	2	17*	1.0	0.5
0	2	18	3.6	4.3
0	2	19	6.5	-5.9
0	3	2	13.2	-11.3
0	3	3	55.7	58.3
0	3	4	16.1	-15.8
0	3	5	33.1	-32.5
0	3	6	28.8	-26.7
0	3	7*	0.6	-0.5
0	3	8	18.9	18.8
0	3	9	50.3	47.9
0	3	10	7.0	6.3
0	3	11	17.3	-18.0
0	3	12	7.4	-6.5
0	3	13	20.5	-20.8
0	3	14	4.8	5.3
0	3	15	14.4	15.1
0	3	16	1.8	1.0
0	3	17*	1.0	0.0
0	3	18	6.6	-7.1
0	3	19	6.3	-6.8
0	4	2	2.3	-2.6
0	4	3	21.4	20.8
0	4	4	36.9	-35.6
0	4	5	19.2	-17.8
0	4	6	76.8	77.5
0	4	7	28.4	-27.0
0	4	8	7.2	7.0
0	4	9	11.6	11.7
0	4	10	24.5	-23.7
0	4	11	3.5	-4.1
0	4	12	20.5	21.0
0	4	13	3.0	3.2
0	4	14*	0.9	1.5
0	4	15	1.9	2.2
0	4	16	7.4	-7.7
0	4	17*	1.0	0.9
0	4	18	13.9	14.2
0	4	19	4.7	-4.8
0	5	2	17.1	15.4
0	5	3	46.9	47.3
0	5	4	9.8	-9.2
0	5	5	19.5	-18.6
0	5	6	14.5	-13.4
0	5	7	17.6	-17.3
0	5	8	4.3	-4.0
0	5	9	16.7	15.7
0	5	10*	0.7	-0.5
0	5	11	4.4	-3.4
0	5	12*	0.8	1.3
0	5	13	6.6	7.3
0	5	14	2.5	-2.6
0	5	15	11.3	11.4
0	5	16	2.6	2.5
0	5	17	4.5	-3.7
0	5	18	2.5	-2.3
0	6	2	8.9	-8.9
0	6	3	6.8	-6.6
0	6	4	33.3	-33.1
0	6	5	1.1	0.5
0	6	6	35.0	34.8
0	6	7	5.2	-5.2
0	6	8	18.5	-18.3
0	6	9	9.0	-9.6
0	6	10	14.1	-14.2
0	6	11	7.0	6.6
0	6	12	11.9	11.9
0	6	13	1.4	-0.1
0	6	14	2.5	-2.5
0	6	15	2.6	-2.8
0	6	16	6.3	-6.4
0	6	17	4.7	5.1
0	6	18	7.5	8.1
0	7	2	25.9	26.4
0	7	3	25.4	24.6
0	7	4	11.4	-10.7
0	7	5	5.5	-5.8
0	7	6	14.9	-14.6
0	7	7	15.9	-15.7
0	7	8	4.4	-4.4
0	7	9	21.7	21.6
0	7	10	1.6	1.7
0	7	11	3.9	-4.2
0	7	12	3.3	3.7
0	7	13	13.2	-13.4
0	7	14*	0.9	1.3
0	7	15	9.1	9.6
0	7	16	1.9	2.3
0	7	17	1.7	1.4
0	8	2	16.2	-16.3
0	8	3	3.3	-2.6
0	8	4	3.7	4.2
0	8	5	22.9	-22.7
0	8	6	50.3	50.7
0	8	7	2.2	1.8
0	8	8	9.0	-8.9
0	8	9	5.8	6.1
0	8	10	3.5	-2.8
0	8	11	6.1	6.5
0	8	12	9.9	9.6
0	8	13	4.2	-3.7
0	8	14	6.9	-7.7
0	8	15*	1.0	-1.3
0	8	16*	1.0	-1.8
0	9	2*	0.3	-0.4
0	9	3	12.2	11.4
0	9	4	9.0	-8.9
0	9	5	17.2	17.0
0	9	6	8.0	-7.6
0	9	7	4.9	4.9
0	9	8	3.1	3.2
0	9	9	11.8	12.0
0	9	10	1.5	1.3
0	9	11	1.8	-1.5
0	9	12	6.2	-6.0
0	9	13	11.3	-10.7
0	9	14	2.0	2.3
0	10	2	14.8	-16.4
0	10	3	1.5	1.4
0	10	4	12.1	-11.8
0	10	5	4.0	-4.1
0	10	6	20.6	20.6
0	10	7	5.9	-5.7
0	10	8	7.9	-7.5
0	10	9	2.0	2.4
0	10	10	6.9	-6.8
0	10	11	4.8	4.6
0	10	12	10.1	10.2
0	10	13	7.9	-7.6
0	11	2*	0.4	0.3
0	11	3	14.4	14.6
0	11	4	3.1	3.4
0	11	5*	0.6	-0.5
0	11	6	7.2	-7.0
0	11	7	8.2	-7.9
0	11	8	1.2	-1.0
0	11	9	5.4	5.6
0	11	10	4.0	3.9
0	11	11*	0.9	-0.7
0	12	2	2.1	-2.5
0	12	3*	0.4	0.4
0	12	4	3.0	3.0
0	12	5*	0.6	0.8
0	12	6	6.4	6.2
0	12	7	2.3	-2.6
0	12	8	1.2	-1.4
0	13	2	0.7	-0.9
0	13	3	10.0	10.2
0	13	4	6.5	-5.8
1	0	0	27.6	-24.4
1	0	2	41.0	41.2
1	0	4	86.2	-87.3
1	0	6	5.0	-4.6
1	0	8	57.5	56.9
1	0	10	36.6	-38.2
1	0	12	38.0	-38.5
1	0	14	11.2	12.5
1	0	16	7.9	-8.0
1	0	18*	1.1	-0.4
1	1	0	41.3	40.9
1	1	1	17.6	-17.7
1	1	2	29.7	28.9
1	1	3	23.3	22.0
1	1	4	37.2	-36.0
1	1	5	30.9	29.3
1	1	6	6.2	4.2
1	1	7	12.6	-12.4
1	1	8*	0.7	0.7
1	1	9	2.2	-1.7
1	1	10	10.7	11.1
1	1	11	24.9	-25.0
1	1	12	13.6	12.5
1	1	13	8.8	-9.1
1	1	14*	0.9	-0.3
1	1	15	1.8	1.5
1	1	16	3.2	-2.2
1	1	17	6.4	7.0
1	1	18	5.3	5.2
1	2	0	20.5	-19.9
1	2	1	26.6	25.0
1	2	2	47.3	47.1
1	2	3	23.3	-22.1
1	2	4	8.1	-3.8
1	2	5	42.9	-42.2
1	2	6	18.8	-18.7
1	2	7*	0.7	2.4
1	2	8	19.1	17.3
1	2	9	10.9	-11.1
1	2	10	9.8	-7.9
1	2	11	14.7	14.2
1	2	12	15.7	-15.5
1	2	13	9.2	9.6
1	2	14	8.7	8.1
1	2	15	5.0	-5.3
1	2	16	2.8	-2.8
1	2	17*	1.1	-0.9
1	2	18	3.7	-3.5
1	3	0	61.0	-63.7
1	3	1	8.9	-8.8
1	3	2	23.6	23.1
1	3	3	33.8	-32.0
1	3	4	40.5	-37.7
1	3	5	3.7	4.3
1	3	6	14.9	-12.9
1	3	7	12.5	-12.1
1	3	8	2.9	2.6
1	3	9	3.0	2.6
1	3	10*	0.8	-0.1
1	3	11	5.9	4.9
1	3	12	12.5	-12.5
1	3	13	15.1	-15.2
1	3	14*	1.0	-1.4
1	3	15*	1.0	0.1
1	3	16*	1.0	-0.4
1	3	17	3.5	4.1
1	3	18	3.1	3.2
1	4	0	23.0	21.5
1	4	1	28.7	28.0
1	4	2	19.0	18.8
1	4	3	23.4	22.2
1	4	4	39.3	-39.2
1	4	5	36.7	-35.4
1	4	6	4.8	-3.1
1	4	7	9.0	-9.0
1	4	8	13.9	13.3
1	4	9	4.8	5.1
1	4	10	22.1	-22.3
1	4	11	2.8	2.8
1	4	12	10.7	-11.8
1	4	13	3.8	-4.9
1	4	14	7.3	7.4
1	4	15	1.7	-1.0
1	4	16	3.0	-3.2
1	4	17	2.3	2.5
1	5	0	3.3	-3.7
1	5	1	14.3	-14.2
1	5	2	4.3	4.7
1	5	3	8.7	-8.2
1	5	4*	0.5	0.1
1	5	5	9.7	10.0
1	5	6	6.4	-6.7
1	5	7	2.1	-2.7
1	5	8	2.6	3.0
1	5	9	10.0	-10.4
1	5	10	11.5	12.8
1	5	11	6.0	5.2
1	5	12	5.7	-6.4
1	5	13	11.9	-13.0
1	5	14*	1.0	0.4
1	5	15	2.0	-2.2
1	5	16	3.6	3.4
1	5	17*	1.1	-0.6
1	6	0	9.2	9.1
1	6	1	8.4	-8.0
1	6	2	27.4	26.4
1	6	3	21.6	-21.9
1	6	4	4.2	-2.8
1	6	5	3.0	2.8
1	6	6	4.5	-4.5
1	6	7	7.7	-7.5
1	6	8	13.6	13.2
1	6	9*	0.8	-0.7
1	6	10	14.9	-16.0
1	6	11	7.1	8.4
1	6	12	7.5	-8.2
1	6	13*	0.9	0.8
1	6	14	7.4	7.6
1	6	15*	1.0	-1.7
1	6	16*	1.1	0.1
1	7	0	9.5	8.8
1	7	1	22.1	-21.1
1	7	2	5.4	4.6
1	7	3	11.7	11.6
1	7	4	11.3	-11.4
1	7	5	2.1	1.2
1	7	6	39.7	-38.8
1	7	7	15.0	-14.4
1	7	8	4.8	-4.8
1	7	9*	0.8	-0.1
1	7	10	12.9	13.3
1	7	11	8.7	8.8
1	7	12*	0.9	-1.7
1	7	13	7.3	-7.6
1	7	14*	1.0	-1.1
1	7	15*	1.0	0.9
1	8	0	12.2	-12.6
1	8	1	7.0	8.2
1	8	2	16.3	15.7
1	8	3	6.8	-7.3
1	8	4	5.3	-4.7
1	8	5	11.6	-11.4
1	8	6	24.0	-23.8
1	8	7	9.4	-9.8
1	8	8	5.5	5.2
1	8	9	2.0	2.0
1	8	10	6.9	-7.1
1	8	11*	0.9	-0.9
1	8	12*	0.9	0.4
1	8	13	1.5	-1.9
1	8	14	8.2	8.2
1	9	0	6.0	-6.0
1	9	1	14.3	-14.2
1	9	2	11.2	11.3
1	9	3	3.2	3.4
1	9	4	5.2	5.1
1	9	5	7.5	-7.2
1	9	6	13.0	-13.1
1	9	7	12.0	-12.7
1	9	8	3.6	3.6
1	9	9	1.8	1.8
1	9	10*	0.8	-0.9
1	9	11	4.3	4.6
1	9	12*	0.9	-0.4
1	9	13	1.9	1.1
1	10	0	1.5	-1.6
1	10	1	7.1	7.2
1	10	2	8.3	7.9
1	10	3	4.4	-4.3
1	10	4	13.7	-13.6
1	10	5	5.2	5.3
1	10	6	5.6	-5.4
1	10	7	3.4	3.7
1	10	8	14.1	13.7
1	10	9	7.6	-7.2
1	10	10*	0.9	-1.0
1	10	11*	0.9	-0.9
1	10	12	1.5	-1.3
1	11	0	9.7	-10.2
1	11	1	10.9	-11.1
1	11	2	4.3	4.5
1	11	3	5.7	5.7
1	11	4	3.7	-3.5
1	11	5	11.3	10.9
1	11	6	8.8	-8.6
1	11	7	10.0	-9.9
1	11	8	1.2	1.0
1	11	9*	0.8	0.4
1	11	10	4.0	-3.9
1	12	0	7.5	-8.1
1	12	1*	0.4	0.3
1	12	2	4.6	4.2
1	12	3	8.3	-7.9
1	12	4	3.6	-3.5
1	12	5	4.0	-3.5
1	12	6	3.2	-2.7
1	12	7*	0.7	0.2
1	13	0	7.7	-8.1
1	13	1	3.0	-3.1
1	13	2	4.9	4.8
2	0	0	25.1	-23.2
2	0	2	53.8	52.2
2	0	4	44.2	-42.7
2	0	6	8.5	-6.6
2	0	8	28.4	26.9
2	0	10	11.5	-11.5
2	0	12	27.7	-26.8
2	0	14	6.6	7.0
2	0	16	7.0	6.8
2	1	0	29.4	28.1
2	1	1	38.4	36.2
2	1	2	2.7	3.5
2	1	3	49.1	-47.8
2	1	4	11.1	9.3
2	1	5	21.7	20.1
2	1	6	3.2	-3.7
2	1	7	11.1	10.9
2	1	8	13.1	-12.0
2	1	9	40.4	-39.0
2	1	10	14.2	-13.6
2	1	11	16.4	16.7
2	1	12	3.8	-5.3
2	1	13*	1.0	0.1
2	1	14	1.5	-1.0
2	1	15	6.9	-7.4
2	1	16	4.3	4.5
2	1	17	5.4	5.4
2	2	0	53.3	-53.2
2	2	1	4.1	-4.1
2	2	2	29.1	27.3
2	2	3	6.4	5.1
2	2	4	4.6	-1.4
2	2	5	23.6	22.0
2	2	6	19.1	-18.7
2	2	7	3.6	-4.0
2	2	8	12.1	10.7
2	2	9	5.3	-5.7
2	2	10	2.9	3.5
2	2	11	3.9	-3.8
2	2	12	13.8	-13.8
2	2	13	4.9	-5.0
2	2	14	4.4	3.8
2	2	15	5.6	5.3
2	2	16	3.9	4.0
2	2	17	1.8	2.0
2	3	0	2.5	0.8
2	3	1	4.4	-3.5
2	3	2*	0.6	-1.6
2	3	3	62.8	-61.6
2	3	4	55.5	52.2
2	3	5	24.1	23.2
2	3	6	2.9	-2.8
2	3	7	9.0	9.3
2	3	8	4.7	-4.7
2	3	9	19.4	-20.5
2	3	10	3.5	3.5
2	3	11	9.0	8.9
2	3	12*	0.9	0.2
2	3	13*	1.0	0.4
2	3	14*	1.0	0.3
2	3	15	9.2	-9.4
2	3	16	11.2	11.4
2	4	0	28.8	-28.2
2	4	1	8.7	9.0
2	4	2	34.4	32.3
2	4	3	13.7	12.9
2	4	4	15.0	-13.5
2	4	5	16.7	-16.7
2	4	6	35.5	-34.8
2	4	7	8.2	-7.3
2	4	8	22.6	21.7
2	4	9	14.3	15.3
2	4	10	2.3	-2.4
2	4	11	6.8	6.5
2	4	12	15.4	-16.1
2	4	13	5.8	-6.2
2	4	14	9.8	10.1
2	4	15	2.1	2.3
2	4	16*	1.1	1.4
2	5	0	6.7	-6.9
2	5	1	2.7	2.5
2	5	2	3.4	-3.0
2	5	3	28.9	-26.8
2	5	4*	0.6	0.4
2	5	5	20.5	19.3
2	5	6	4.4	-4.4
2	5	7	2.2	1.9
2	5	8	1.7	-1.0
2	5	9	12.4	-12.3
2	5	10	4.3	-4.8
2	5	11*	0.9	-0.2
2	5	12*	1.0	0.6
2	5	13	2.8	2.2
2	5	14	3.8	-4.4
2	5	15	7.3	-8.0
2	6	0	17.3	-16.8
2	6	1	8.2	8.1
2	6	2	16.9	15.5
2	6	3	13.8	13.5
2	6	4	4.5	-4.3
2	6	5*	0.7	0.3
2	6	6	18.8	-18.6
2	6	7	6.3	6.0
2	6	8	13.2	13.2
2	6	9	8.1	-8.9
2	6	10*	0.9	0.8
2	6	11	7.7	-8.2
2	6	12	8.5	-8.8
2	6	13	2.2	1.9
2	6	14	4.0	4.6
2	6	15	2.7	2.2
2	7	0*	0.5	0.7
2	7	1	7.6	-7.2
2	7	2	30.6	30.1
2	7	3	48.4	-47.4
2	7	4	11.4	11.2
2	7	5	27.7	27.2
2	7	6	1.7	2.0
2	7	7	5.6	5.7
2	7	8*	0.8	-0.5
2	7	9	13.4	-13.5
2	7	10*	0.9	-0.1
2	7	11	8.1	8.3
2	7	12*	1.0	-0.1
2	7	13	1.8	-1.1
2	7	14*	1.1	0.0
2	8	0	17.3	-17.7
2	8	1	12.6	13.2
2	8	2	1.9	2.0
2	8	3	23.0	24.7
2	8	4	9.2	-8.8
2	8	5*	0.7	-0.6
2	8	6	8.8	-8.8
2	8	7	4.0	-3.7
2	8	8	4.8	4.5
2	8	9	2.2	2.4
2	8	10	1.7	1.9
2	8	11	3.8	-4.0
2	8	12	3.6	-3.7
2	8	13*	1.0	0.2
2	9	0	6.1	-6.4
2	9	1	8.1	7.6
2	9	2	3.1	-3.0
2	9	3	30.6	-30.1
2	9	4	1.8	-1.3
2	9	5	5.5	6.0
2	9	6	3.2	-3.3
2	9	7	2.6	2.3
2	9	8	6.2	-6.5
2	9	9	11.5	-11.9
2	9	10	8.1	8.5
2	9	11	8.9	9.4
2	10	0	7.6	-7.5
2	10	1	3.8	3.5
2	10	2	4.6	4.9
2	10	3	2.1	-2.6
2	10	4	8.0	-8.2
2	10	5	5.2	-4.9
2	10	6	6.5	-6.8
2	10	7	3.8	-4.0
2	10	8	5.9	6.1
2	10	9	5.9	5.5
2	10	10*	0.9	-0.2
2	11	0	8.8	8.7
2	11	1	3.0	-2.6
2	11	2*	0.6	0.6
2	11	3	10.2	-10.0
2	11	4	1.2	0.6
2	11	5	5.6	5.4
2	11	6	3.2	3.0
2	11	7	2.2	-2.3
2	11	8*	0.9	-0.7
2	12	0	12.7	-12.6
2	12	1	4.1	3.6
2	12	2*	0.6	0.5
2	12	3	4.1	3.6
2	12	4	1.5	1.6
2	12	5	2.1	2.1
3	0	0	19.9	-17.1
3	0	2	43.4	-41.1
3	0	4	28.1	26.1
3	0	6	6.5	-5.5
3	0	8	26.8	25.4
3	0	10	24.4	24.1
3	0	12	7.4	-6.7
3	0	14	4.8	-5.0
3	1	0	21.8	20.3
3	1	1	14.7	14.5
3	1	2	38.0	35.8
3	1	3	11.9	-10.3
3	1	4	14.6	-15.5
3	1	5	30.2	-29.0
3	1	6	2.5	-2.4
3	1	7	23.9	22.7
3	1	8	8.3	9.1
3	1	9	30.0	30.5
3	1	10*	0.9	0.6
3	1	11	9.9	-10.3
3	1	12	2.8	2.1
3	1	13	3.8	4.0
3	1	14*	1.1	2.2
3	1	15*	1.1	0.8
3	2	0	1.8	-1.4
3	2	1	5.5	3.9
3	2	2	28.4	-25.8
3	2	3	11.3	9.8
3	2	4	22.7	22.6
3	2	5	1.8	-1.7
3	2	6	5.1	-5.6
3	2	7	6.5	6.4
3	2	8	8.3	-7.1
3	2	9	4.9	5.0
3	2	10	10.7	10.9
3	2	11	6.8	-6.5
3	2	12*	1.0	-1.1
3	2	13	1.7	2.0
3	2	14	5.2	-6.2
3	2	15	3.5	-4.3
3	3	0	20.8	-20.1
3	3	1	44.8	42.3
3	3	2	23.1	21.2
3	3	3	5.3	-6.3
3	3	4	9.5	9.3
3	3	5	18.1	-17.6
3	3	6	7.8	-7.9
3	3	7	22.5	22.5
3	3	8	9.5	-10.0
3	3	9	1.5	1.7
3	3	10	2.1	2.2
3	3	11	10.5	-11.1
3	3	12	2.4	2.5
3	3	13	7.6	8.2
3	3	14*	1.1	-1.2
3	3	15	5.4	5.2
3	4	0	1.8	0.9
3	4	1	16.6	15.9
3	4	2	3.7	-3.5
3	4	3	17.0	15.9
3	4	4	14.5	13.4
3	4	5	1.5	-1.8
3	4	6	3.5	4.7
3	4	7	8.6	-8.9
3	4	8	1.5	0.1
3	4	9	7.1	7.2
3	4	10	16.8	17.2
3	4	11	2.2	-2.0
3	4	12*	1.0	0.5
3	4	13	2.1	-2.6
3	4	14	2.2	-2.8
3	5	0	17.6	17.0
3	5	1	20.9	19.9
3	5	2	16.5	15.6
3	5	3	11.4	11.1
3	5	4	8.0	7.7
3	5	5	18.5	-18.3
3	5	6*	0.8	0.5
3	5	7	19.9	20.4
3	5	8	6.0	-6.8
3	5	9	5.7	7.0
3	5	10	3.7	3.8
3	5	11	7.0	-6.7
3	5	12	2.9	2.6
3	5	13	4.8	4.6
3	5	14*	1.1	-0.6
3	6	0	13.1	-13.2
3	6	1	16.8	16.8
3	6	2	23.6	-22.6
3	6	3	10.6	10.4
3	6	4	2.7	2.5
3	6	5*	0.8	0.2
3	6	6	1.5	1.1
3	6	7	4.0	-4.7
3	6	8	4.0	-3.8
3	6	9	3.1	3.5
3	6	10	13.3	14.2
3	6	11	1.6	1.7
3	6	12	2.9	-2.5
3	6	13*	1.1	-0.2
3	7	0	9.2	9.4
3	7	1	6.4	5.9
3	7	2	0.6	0.9
3	7	3	4.5	3.9
3	7	4	5.3	4.9
3	7	5	7.6	-7.3
3	7	6*	0.8	0.6
3	7	7	11.0	11.3
3	7	8	2.2	-2.1
3	7	9	2.2	-3.0
3	7	10	3.6	4.2
3	7	11	7.9	-8.5
3	7	12*	1.0	-1.2
3	8	0	4.2	-4.0
3	8	1	3.2	3.5
3	8	2	4.3	4.1
3	8	3	13.1	13.5
3	8	4	25.8	25.1
3	8	5	1.8	-2.1
3	8	6	4.0	-3.9
3	8	7	2.6	-2.6
3	8	8	11.3	-11.3
3	8	9	2.2	2.1
3	8	10	6.6	7.1
3	8	11*	1.0	1.3
3	9	0	1.8	-1.7
3	9	1	13.2	12.7
3	9	2*	0.7	-1.0
3	9	3	14.8	14.9
3	9	4	13.2	13.0
3	9	5	7.8	-7.2
3	9	6	7.6	7.3
3	9	7	1.3	1.2
3	9	8*	0.9	0.9
3	9	9	1.8	1.5
3	10	0	8.2	-8.0
3	10	1	9.1	8.5
3	10	2	8.0	-7.7
3	10	3	13.9	13.6
3	10	4	13.8	14.2
3	10	5	6.2	-5.8
3	10	6	4.6	-4.6
3	10	7	4.8	4.7
3	10	8	7.3	-7.3
3	11	0	4.7	4.4
3	11	1	2.7	2.9
3	11	2	2.6	2.7
3	11	3	2.5	-2.6
3	11	4	1.6	-1.3
3	11	5	3.3	-3.4
3	12	0*	0.7	0.2
3	12	1	2.2	-2.0
3	12	2	3.9	-4.1
4	0	0	24.5	23.3
4	0	2	9.4	-8.3
4	0	4	10.5	-10.7
4	0	6	13.3	13.4
4	0	8	18.3	-19.3
4	0	10	2.9	2.3
4	0	12	6.5	7.5
4	1	0	1.3	2.5
4	1	1	26.2	24.7
4	1	2	2.3	-2.1
4	1	3	11.4	10.3
4	1	4	7.8	-8.0
4	1	5	19.1	-18.6
4	1	6	3.4	3.3
4	1	7	13.2	13.0
4	1	8	9.2	9.4
4	1	9	8.8	8.9
4	1	10	3.9	4.0
4	1	11	7.5	-7.4
4	1	12	3.3	-3.7
4	1	13	2.0	1.6
4	2	0	36.1	32.7
4	2	1	19.9	-18.3
4	2	2	6.6	-5.8
4	2	3*	0.8	1.7
4	2	4*	0.8	-0.7
4	2	5	10.2	9.7
4	2	6	24.6	24.1
4	2	7	6.2	5.8
4	2	8	6.1	-5.6
4	2	9	1.7	-2.0
4	2	10	4.9	5.0
4	2	11*	1.1	1.4
4	2	12	8.0	8.0
4	2	13	6.9	-7.1
4	3	0	3.1	-2.6
4	3	1	12.5	12.2
4	3	2	13.3	-12.7
4	3	3	1.4	0.7
4	3	4*	0.8	-1.1
4	3	5	11.3	-10.7
4	3	6	2.9	2.3
4	3	7	15.5	15.5
4	3	8	1.7	-2.0
4	3	9	11.4	11.6
4	3	10	4.4	5.0
4	3	11	8.4	-8.6
4	3	12*	1.1	-1.0
4	4	0	13.6	13.0
4	4	1	8.0	-7.5
4	4	2	27.9	-27.6
4	4	3	4.6	4.0
4	4	4	7.0	7.2
4	4	5	2.1	2.3
4	4	6	9.6	10.2
4	4	7	2.2	-1.3
4	4	8	6.3	-6.5
4	4	9	3.0	-3.3
4	4	10	1.9	1.9
4	4	11	4.1	3.9
4	4	12*	1.1	1.6
4	5	0	7.0	-7.0
4	5	1	18.9	18.6
4	5	2	6.8	6.9
4	5	3	17.6	17.4
4	5	4	2.1	-2.2
4	5	5	15.4	-15.8
4	5	6	1.3	-0.8
4	5	7	4.8	-4.9
4	5	8	5.0	5.2
4	5	9	6.3	6.8
4	5	10*	1.0	0.3
4	5	11	2.5	-3.2
4	6	0	35.1	34.8
4	6	1	15.3	-15.1
4	6	2	16.0	-15.7
4	6	3	7.3	7.5
4	6	4	4.5	4.9
4	6	5	1.4	0.8
4	6	6	9.9	10.0
4	6	7	1.8	1.9
4	6	8	3.4	-3.8
4	6	9	3.2	4.0
4	6	10	1.9	2.1
4	6	11	1.6	-1.1
4	7	0	17.8	-17.5
4	7	1	19.7	19.3
4	7	2	2.0	2.0
4	7	3	1.2	1.3
4	7	4*	0.9	-0.3
4	7	5	10.3	-9.9
4	7	6*	0.9	-0.3
4	7	7	7.3	7.6
4	7	8	5.8	6.5
4	7	9	2.3	2.5
4	7	10	1.9	-1.7
4	8	0	13.6	14.1
4	8	1	9.3	-9.7
4	8	2	11.6	-11.8
4	8	3	3.6	-3.8
4	8	4	2.3	-2.7
4	8	5	4.5	4.0
4	8	6	7.8	8.3
4	8	7	4.5	-4.2
4	8	8	4.6	-4.2
4	9	0	2.5	-2.4
4	9	1	6.6	6.5
4	9	2	3.1	2.6
4	9	3	3.7	3.7
4	9	4	1.9	1.8
4	9	5	6.4	-6.7
4	9	6*	0.9	-1.0
4	9	7	6.0	6.4
4	10	0	13.0	12.4
4	10	1	4.4	4.2
4	10	2	1.5	-2.0
4	10	3	1.4	-1.3
4	10	4	3.9	4.3
4	10	5	1.4	1.5
4	11	0	2.2	2.9
4	11	1	7.5	7.7
4	11	2	4.1	4.2
5	0	0	30.9	29.6
5	0	2	2.7	2.1
5	0	4	19.1	-17.9
5	0	6	11.2	-10.8
5	0	8	6.8	6.4
5	0	10	2.3	-2.9
5	1	0	3.2	-2.7
5	1	1	19.8	-20.1
5	1	2*	0.9	0.7
5	1	3	13.7	13.4
5	1	4	6.0	-5.9
5	1	5	2.1	-1.6
5	1	6	11.9	-11.4
5	1	7	20.6	-21.2
5	1	8*	1.0	1.5
5	1	9	4.4	4.7
5	1	10*	1.1	0.4
5	1	11	4.5	4.9
5	2	0	19.1	18.7
5	2	1*	0.9	1.3
5	2	2	13.5	13.8
5	2	3	5.1	5.5
5	2	4	24.9	-25.0
5	2	5	4.3	-4.6
5	2	6	8.1	-8.4
5	2	7	9.2	-9.6
5	2	8	6.9	7.2
5	2	9*	1.1	1.1
5	2	10	7.5	-8.0
5	3	0	9.0	-8.8
5	3	1	18.4	-18.2
5	3	2	2.3	-2.2
5	3	3	5.7	5.5
5	3	4	7.4	7.4
5	3	5*	1.0	-1.7
5	3	6*	1.0	0.2
5	3	7	12.3	-13.2
5	3	8	4.3	4.7
5	3	9	4.6	4.6
5	3	10*	1.1	-0.1
5	4	0	4.8	4.4
5	4	1	2.0	-1.9
5	4	2	12.5	12.7
5	4	3*	0.9	1.1
5	4	4	15.8	-16.5
5	4	5	6.5	6.9
5	4	6*	1.0	1.8
5	4	7	2.2	-1.5
5	4	8	5.2	5.3
5	4	9*	1.1	-0.7
5	4	10	6.9	-7.8
5	5	0	14.9	-14.3
5	5	1	14.9	-14.7
5	5	2	2.8	-3.1
5	5	3	5.8	6.0
5	5	4	2.5	2.5
5	5	5*	1.0	0.4
5	5	6	2.8	-2.1
5	5	7	13.7	-14.7
5	5	8*	1.1	-0.2
5	5	9	6.3	6.8
5	6	0*	0.9	1.0
5	6	1	4.7	-4.7
5	6	2	7.5	7.5
5	6	3*	0.9	1.3
5	6	4	13.1	-13.3
5	6	5*	1.0	0.1
5	6	6	3.8	4.2
5	6	7	4.6	-5.3
5	6	8	2.9	3.2
5	7	0	3.1	3.2
5	7	1	15.4	-15.7
5	7	2	5.3	5.3
5	7	3	3.9	4.3
5	7	4	3.9	-3.7
5	7	5	6.0	6.2
5	7	6	4.6	-4.7
5	7	7	9.3	-10.2
5	8	0*	0.9	0.1
5	8	1	6.2	-6.2
5	8	2	6.4	6.2
5	8	3	4.1	-4.4
5	8	4	2.8	-3.5
5	8	5*	1.0	-0.9
5	8	6	3.5	3.8
5	9	0	11.7	-11.5
5	9	1	16.2	-16.5
5	9	2*	0.9	0.7
5	9	3	5.8	6.1
5	9	4	3.7	-3.3
5	10	0*	0.9	0.2
5	10	1	8.5	-8.6
5	10	2	3.8	-4.2
6	0	0	10.4	-10.1
6	0	2	8.4	8.6
6	0	4	6.4	-6.2
6	0	6*	1.1	1.9
6	0	8	5.2	5.4
6	1	0*	0.9	0.8
6	1	1	2.8	3.1
6	1	2	3.2	2.6
6	1	3	6.9	-6.8
6	1	4	2.2	1.9
6	1	5	5.4	5.8
6	1	6	2.6	3.1
6	1	7	4.2	-4.0
6	1	8*	1.1	-0.4
6	2	0	3.3	-3.1
6	2	1	2.2	2.4
6	2	2	9.3	9.4
6	2	3	2.4	-2.1
6	2	4	14.2	-14.5
6	2	5	2.4	-2.0
6	2	6	6.5	-6.8
6	2	7*	1.1	-0.8
6	3	0	5.2	-5.1
6	3	1	3.9	-3.8
6	3	2*	1.0	-0.7
6	3	3	12.3	-12.4
6	3	4	4.3	-4.5
6	3	5*	1.1	0.6
6	3	6	2.1	0.5
6	3	7	2.4	-2.9
6	4	0	1.7	1.5
6	4	1	4.1	4.2
6	4	2	5.6	5.9
6	4	3	7.7	-8.1
6	4	4	5.9	-5.9
6	4	5	6.7	-7.0
6	4	6	3.6	-3.8
6	4	7*	1.1	0.2
6	5	0	4.1	-3.6
6	5	1	4.1	-4.5
6	5	2*	1.0	-0.4
6	5	3	3.9	-4.7
6	5	4*	1.0	0.4
6	5	5	5.0	5.4
6	5	6*	1.1	-1.6
6	6	0*	1.0	-1.4
6	6	1	1.9	-1.7
6	6	2	8.4	8.4
6	6	3	1.5	1.2
6	6	4	3.8	-3.9
6	6	5*	1.1	-1.4
6	7	0	1.8	-2.0
6	7	1	3.1	-3.2
6	7	2	4.3	-4.2
6	7	3	3.6	-3.9
6	7	4	2.0	1.5
6	8	0*	1.0	-0.7
6	8	1	2.4	2.4
6	8	2	6.0	6.4
6	9	0	2.0	2.7
7	0	0	14.2	-14.1
7	0	2*	1.1	-0.4
7	0	4	11.0	11.5
7	1	0*	1.0	0.6
7	1	1	12.2	12.3
7	1	2*	1.1	0.0
7	1	3	2.4	-2.6
7	1	4	4.1	3.9
7	1	5*	1.1	-1.1
7	2	0	9.6	-9.9
7	2	1	3.2	-3.0
7	2	2	9.5	9.3
7	2	3	3.9	4.0
7	2	4	14.0	15.2
7	3	0*	1.0	1.1
7	3	1	12.3	12.5
7	3	2*	1.1	1.0
7	3	3*	1.1	1.1
7	3	4	4.4	4.6
7	4	0	9.1	-9.9
7	4	1	2.9	-2.8
7	4	2*	1.1	1.7
7	4	3*	1.1	-0.2
7	5	0*	1.0	-0.8
7	5	1	7.4	7.9
7	5	2	1.7	-1.3
7	6	0	6.7	-6.9
7	6	1*	1.1	1.6
8	0	0	6.0	5.9
8	1	0*	1.1	-0.6
8	2	0	4.4	4.6
8	3	0	4.1	3.9
-1	0	2	3.6	-10.0
-1	0	4	35.1	-33.6
-1	0	6	16.5	16.2
-1	0	8	8.3	-6.6
-1	0	10	3.2	-4.3
-1	0	12*	0.8	-0.7
-1	0	14	9.4	10.4
-1	0	16	1.6	2.5
-1	0	18	5.5	5.7
-1	0	20	10.0	-11.0
-1	1	1	8.2	-6.9
-1	1	2	28.7	-27.6
-1	1	3	5.7	-5.9
-1	1	4	11.4	-10.0
-1	1	5	53.8	-57.3
-1	1	6	24.2	-23.1
-1	1	7	65.2	67.1
-1	1	8	2.7	1.5
-1	1	9	8.4	8.3
-1	1	10	24.3	23.6
-1	1	11	23.9	-23.1
-1	1	12	3.4	2.2
-1	1	13	24.4	23.9
-1	1	14	23.1	-22.8
-1	1	15	12.6	11.9
-1	1	16	4.0	-3.2
-1	1	17	8.9	-8.6
-1	1	18*	1.0	0.9
-1	1	19	5.8	5.4
-1	1	20	1.7	-1.2
-1	1	21*	1.1	0.7
-1	2	1	55.8	-55.1
-1	2	2	36.7	35.5
-1	2	3	30.6	-29.0
-1	2	4	43.8	44.4
-1	2	5	13.2	12.4
-1	2	6	1.6	0.7
-1	2	7	58.1	57.3
-1	2	8	4.4	1.6
-1	2	9	2.8	2.1
-1	2	10	14.2	12.7
-1	2	11	4.7	4.8
-1	2	12	1.6	2.2
-1	2	13	23.4	-22.6
-1	2	14	20.9	21.2
-1	2	15	4.0	-3.7
-1	2	16	15.1	15.1
-1	2	17	5.3	4.9
-1	2	18	1.7	-0.3
-1	2	19*	1.1	1.2
-1	2	20	4.2	-4.3
-1	2	21*	1.1	-0.5
-1	3	1	73.8	75.6
-1	3	2	6.5	6.2
-1	3	3*	0.4	0.5
-1	3	4	36.0	-37.0
-1	3	5	48.0	-49.1
-1	3	6	26.0	25.3
-1	3	7	19.9	19.6
-1	3	8	32.9	30.4
-1	3	9	15.7	16.2
-1	3	10	5.5	-5.9
-1	3	11	22.0	-21.9
-1	3	12	10.1	10.6
-1	3	13	14.1	13.8
-1	3	14	3.4	-1.8
-1	3	15	20.5	22.2
-1	3	16*	0.9	-1.2
-1	3	17	5.9	-6.0
-1	3	18*	1.0	0.8
-1	3	19*	1.1	0.6
-1	3	20*	1.1	-0.3
-1	4	1	24.7	24.4
-1	4	2	58.6	-60.9
-1	4	3	30.3	30.0
-1	4	4	14.3	14.0
-1	4	5	17.7	-16.6
-1	4	6	5.0	5.4
-1	4	7	11.6	10.3
-1	4	8	14.9	-14.0
-1	4	9	3.6	3.2
-1	4	10	10.7	11.2
-1	4	11	3.5	3.7
-1	4	12*	0.8	-0.0
-1	4	13	5.8	-6.6
-1	4	14	8.4	-7.6
-1	4	15	5.3	6.0
-1	4	16	8.7	9.3
-1	4	17	1.9	2.3
-1	4	18*	1.0	-1.2
-1	4	19*	1.1	0.9
-1	4	20*	1.1	-1.3
-1	5	1	9.3	9.7
-1	5	2	12.1	-10.0
-1	5	2	18.1	-17.4
-1	5	4	4.3	-4.4
-1	5	5	13.6	13.0
-1	5	6	11.6	-11.0
-1	5	7	8.3	8.2
-1	5	8	8.2	8.2
-1	5	9	4.1	-4.6
-1	5	10	2.5	2.9
-1	5	11	9.5	-9.4
-1	5	12	4.1	-3.7
-1	5	13	15.0	14.1
-1	5	14	2.2	-2.7
-1	5	15	6.8	6.5
-1	5	16*	1.0	-0.2
-1	5	17	6.1	-6.4
-1	5	18*	1.0	-0.3
-1	5	19	3.0	3.0
-1	6	1	40.2	-37.9
-1	6	2	28.0	-26.7
-1	6	3	1.1	2.1
-1	6	4	10.7	10.9
-1	6	5	4.0	-4.7
-1	6	6	3.8	-3.0
-1	6	7	2.6	-1.7
-1	6	8	14.8	15.4
-1	6	9	30.3	30.9
-1	6	10	22.1	22.2
-1	6	11	1.7	1.3
-1	6	12	4.3	4.9
-1	6	13	14.7	-15.7
-1	6	14	8.4	-8.0
-1	6	15*	0.9	1.6
-1	6	16	7.2	7.5
-1	6	17*	1.0	-0.2
-1	6	18	1.5	0.4
-1	6	19	3.2	-3.4
-1	7	1	33.1	32.0
-1	7	2	0.9	0.6
-1	7	3	10.3	10.2
-1	7	4	1.8	1.8
-1	7	5	32.9	-32.2
-1	7	6	7.5	7.5
-1	7	7	13.8	13.3
-1	7	8	24.1	23.5
-1	7	9	22.2	22.4
-1	7	10	12.6	12.8
-1	7	11	11.9	-12.1
-1	7	12	5.3	-5.4
-1	7	13	11.2	11.2
-1	7	14	3.7	-4.3
-1	7	15	5.9	6.6
-1	7	16	4.6	-4.5
-1	7	17	6.4	-6.2
-1	7	18	2.7	2.9
-1	8	1	4.2	4.9
-1	8	2	4.7	-4.3
-1	8	3	6.2	5.6
-1	8	4	12.8	11.9
-1	8	5	5.4	-5.4
-1	8	6	12.7	-12.9
-1	8	7	3.2	2.1
-1	8	8	2.3	-1.5
-1	8	9	22.7	22.9
-1	8	10	2.3	2.6
-1	8	11*	0.8	0.3
-1	8	12	5.2	5.1
-1	8	13	2.5	-3.1
-1	8	14	3.1	-3.7
-1	8	15	2.0	-1.9
-1	8	16*	1.0	-1.0
-1	8	17*	1.0	-0.6
-1	9	1	9.5	9.5
-1	9	2	3.7	4.3
-1	9	3	6.0	6.1
-1	9	4	13.6	-13.5
-1	9	5	15.6	-15.1
-1	9	6	14.1	14.1
-1	9	7	10.8	11.1
-1	9	8	3.3	3.3
-1	9	9	3.6	3.0
-1	9	10	8.5	-8.6
-1	9	11	8.7	-8.9
-1	9	12*	0.8	-0.3
-1	9	13	6.7	7.0
-1	9	14*	0.9	1.3
-1	9	15	3.4	-3.6
-1	9	16*	1.0	-1.6
-1	10	1	10.4	11.3
-1	10	2	1.6	2.3
-1	10	3	8.5	9.0
-1	10	4	12.2	12.1
-1	10	5	1.7	-2.1
-1	10	6	3.1	3.0
-1	10	7	13.0	-12.9
-1	10	8*	0.4	-0.2
-1	10	9	3.8	3.4
-1	10	10	7.7	8.0
-1	10	11	4.7	4.3
-1	10	12	1.6	1.2
-1	10	13*	0.9	0.4
-1	10	14	3.2	-3.6
-1	11	1*	0.4	0.4
-1	11	2	12.3	13.2
-1	11	3	6.8	7.2
-1	11	4	4.5	-4.1
-1	11	5	5.1	-4.7
-1	11	6	4.6	4.3
-1	11	7	11.5	11.8
-1	11	8	1.4	-1.8
-1	11	9	8.6	8.2
-1	11	10	2.6	2.7
-1	11	11	3.6	-3.1
-1	11	12	8.3	8.2
-1	12	1	2.6	3.7
-1	12	2	2.6	-3.0
-1	12	3	3.6	3.9
-1	12	4	6.5	6.7
-1	12	5	0.8	0.9
-1	12	6	1.0	-1.0
-1	12	7	2.1	1.6
-1	12	8	6.3	-6.5
-1	12	9	6.7	6.0
-1	13	1	2.4	2.7
-1	13	2	1.3	1.6
-1	13	3	1.5	1.0
-1	13	4	5.9	-5.6
-1	13	5	6.8	-6.6
-2	0	2	120.7	-124.8
-2	0	4	14.4	15.0
-2	0	6	35.8	-34.7
-2	0	8	1.4	-0.5
-2	0	10	67.5	66.9
-2	0	12	24.1	-24.2
-2	0	14	24.4	-23.6
-2	0	16	21.9	22.7
-2	0	18	11.0	-11.8
-2	0	20*	1.1	-1.0
-2	0	22	11.2	11.2
-2	1	1	35.4	36.5
-2	1	2	96.9	101.2
-2	1	3	164.5	-174.4
-2	1	4	76.8	76.7
-2	1	5*	0.5	-0.0
-2	1	6	34.0	-31.9
-2	1	7	35.0	34.8
-2	1	8	10.2	-9.8
-2	1	9	16.7	-16.2
-2	1	10	23.2	21.5
-2	1	11	4.6	4.2
-2	1	12	5.1	-5.0
-2	1	13	22.5	21.7
-2	1	14	13.1	12.5
-2	1	15	21.8	-20.6
-2	1	16	8.3	8.4
-2	1	17	7.3	-7.1
-2	1	18	1.9	2.6
-2	1	19	4.1	3.9
-2	1	20*	1.1	-0.4
-2	1	21	2.7	2.0
-2	1	22	2.2	1.4
-2	2	1	7.9	-7.4
-2	2	2	53.9	-53.5
-2	2	3	30.0	28.6
-2	2	4	17.1	17.6
-2	2	5	6.5	-5.9
-2	2	6	20.1	-19.6
-2	2	7	1.7	2.2
-2	2	8	3.3	-2.9
-2	2	9	28.7	27.0
-2	2	10	16.2	13.5
-2	2	11	20.6	-19.6
-2	2	12	25.3	-23.7
-2	2	13	4.1	-3.2
-2	2	14	1.9	0.7
-2	2	15	6.7	6.0
-2	2	16	17.0	16.8
-2	2	17*	0.9	1.3
-2	2	18	14.8	-14.2
-2	2	19*	1.0	0.9
-2	2	20*	1.1	-0.9
-2	2	21	1.7	2.5
-2	3	1	67.6	68.1
-2	3	2	3.6	3.4
-2	3	3	77.9	-80.5
-2	3	4	28.1	-26.7
-2	3	5	38.0	-36.2
-2	3	6	1.1	-1.8
-2	3	7	58.3	57.6
-2	3	8	3.3	-2.9
-2	3	9	32.8	-31.0
-2	3	10	1.7	-1.4
-2	3	11	16.3	-16.3
-2	3	12	9.3	-9.1
-2	3	13	22.7	22.5
-2	3	14	6.5	6.0

Table 1 (*cont.*)

-2	3	15	9.9	-10.2
-2	3	16	10.3	-10.6
-2	3	17*	1.0	-0.6
-2	3	18	1.6	-1.8
-2	3	19	7.8	7.7
-2	3	20	2.9	-2.6
-2	3	21	4.9	-5.0
-2	4	1	4.2	3.9
-2	4	2	18.8	-18.3
-2	4	3	12.8	-11.4
-2	4	4	2.3	3.5
-2	4	5	23.2	-20.8
-2	4	6	34.2	-33.3
-2	4	7	6.4	6.0
-2	4	8	10.1	-9.1
-2	4	9	23.4	21.8
-2	4	10	23.6	22.9
-2	4	11	9.9	9.4
-2	4	12	7.5	-6.8
-2	4	13*	0.8	0.7
-2	4	14	5.5	-5.8
-2	4	15	12.3	-13.1
-2	4	16	12.2	12.4
-2	4	17	6.4	-6.6
-2	4	18	5.1	-5.1
-2	4	19*	1.0	1.2
-2	4	20	6.6	-6.9
-2	4	21	5.3	4.9
-2	5	1*	0.5	1.6
-2	5	2	19.5	17.4
-2	5	3	45.3	-44.7
-2	5	4	6.6	-6.0
-2	5	5	2.7	3.0
-2	5	6	4.7	5.1
-2	5	7	37.3	37.9
-2	5	8	12.6	11.6
-2	5	9	44.9	-44.5
-2	5	10	27.0	26.6
-2	5	11	3.8	3.7
-2	5	12	3.8	4.1
-2	5	13	18.0	17.6
-2	5	14	2.8	-2.4
-2	5	15	12.7	-13.1
-2	5	16	1.5	1.4
-2	5	17*	1.0	-0.5
-2	5	18*	1.0	0.7
-2	5	19	6.4	6.7
-2	5	20*	1.1	-0.8
-2	6	1	27.4	26.1
-2	6	2	9.7	-7.9
-2	6	3	4.1	4.0
-2	6	4	6.1	5.6
-2	6	5	6.9	-7.3
-2	6	6	25.5	-25.6
-2	6	7	7.0	6.0
-2	6	8	4.1	-3.7
-2	6	9	11.6	11.9
-2	6	10	24.0	23.7
-2	6	11	2.2	2.1
-2	6	12	11.6	-11.5
-2	6	13	5.3	-4.9
-2	6	14	6.2	-5.7
-2	6	15	7.0	6.7
-2	6	16	7.3	7.5
-2	6	17	3.7	3.7
-2	6	18	6.9	-7.4
-2	6	19	4.8	-5.1
-2	7	1	22.0	21.8
-2	7	2	10.3	9.8
-2	7	3	22.7	-21.0
-2	7	4	2.1	2.0
-2	7	5	5.9	-5.6
-2	7	6	2.4	-2.5
-2	7	7	25.0	24.3
-2	7	8	5.6	-5.3
-2	7	9	23.9	-23.8
-2	7	10*	0.7	-0.2
-2	7	11	5.8	-5.7
-2	7	12	2.1	-2.5
-2	7	13	5.4	4.6
-2	7	14	8.4	-8.6
-2	7	15	2.7	-2.9
-2	7	16	3.8	3.7
-2	7	17*	1.0	-0.7
-2	7	18*	1.0	0.1
-2	7	19	6.5	6.5
-2	8	1	13.2	12.7
-2	8	2	7.8	-6.9
-2	8	3	1.3	1.7
-2	8	4	28.8	29.3
-2	8	5	1.7	-0.8
-2	8	6	9.9	-9.8
-2	8	7	4.0	3.6
-2	8	8	20.8	-20.2
-2	8	9	3.3	-3.6
-2	8	10	8.0	7.7
-2	8	11	2.3	-2.1
-2	8	12	13.0	-12.8
-2	8	13	1.6	-1.6
-2	8	14	1.6	2.1
-2	8	15	2.8	1.7
-2	8	16	14.2	13.9
-2	8	17*	1.0	0.0
-2	8	18	3.7	-3.9
-2	9	1	12.5	13.0
-2	9	2	12.3	-12.0
-2	9	3	13.7	-13.1
-2	9	4	3.5	4.0
-2	9	5	10.3	10.7
-2	9	6	7.6	7.4
-2	9	7*	0.6	-0.3
-2	9	8	18.9	18.5
-2	9	9	22.5	-22.7
-2	9	10	6.8	6.8
-2	9	11	3.9	3.5
-2	9	12*	0.8	0.7
-2	9	13	7.0	6.7
-2	9	14	4.2	-4.3
-2	9	15	2.2	-2.1
-2	9	16	3.6	3.1
-2	10	1	2.2	-2.3
-2	10	2	1.6	1.1
-2	10	3	7.9	8.1
-2	10	4	18.4	18.4
-2	10	5	3.6	-3.7
-2	10	6	15.3	-15.6
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-2	10	9	15.1	14.6
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-2	10	12	7.4	-7.7
-2	10	13	2.1	-2.0
-2	10	14	3.8	-3.5
-2	10	15	4.5	4.5
-2	11	1	12.9	13.0
-2	11	2	3.7	-3.6
-2	11	3	10.6	-10.7
-2	11	4	7.3	7.0
-2	11	5*	0.6	0.3
-2	11	6	9.7	-9.9
-2	11	7	2.5	2.0
-2	11	8	4.0	3.9
-2	11	9	9.5	-9.7
-2	11	10	3.6	4.2
-2	11	11*	0.8	-0.2
-2	11	12	2.9	-2.5
-2	11	13	7.8	7.6
-2	12	1*	0.5	-1.1
-2	12	2	1.9	2.0
-2	12	3*	0.5	0.5
-2	12	4	10.0	9.4
-2	12	5	2.1	-2.4
-2	12	6	4.9	-5.1
-2	12	7	4.0	3.6
-2	12	8	1.3	-0.7
-2	12	9	1.8	2.0
-2	12	10*	0.8	1.4
-2	13	1	10.0	10.2
-2	13	2	2.2	2.1
-2	13	3	5.6	-5.8
-2	13	4	6.0	5.8
-3	0	2	63.0	61.3
-3	0	4	16.6	-17.3
-3	0	6	1.3	-1.4
-3	0	8	55.1	53.4
-3	0	10	37.0	-34.7
-3	0	12	20.3	-19.2
-3	0	14	8.3	8.0
-3	0	16	6.4	-6.5
-3	0	18*	1.0	-1.7
-3	0	20	6.5	6.1
-3	0	22	2.1	-1.3
-3	1	1	30.4	-29.0
-3	1	2	7.8	8.2
-3	1	3	18.4	16.1
-3	1	4	8.3	7.7
-3	1	5	27.3	27.1
-3	1	6	18.5	-17.0
-3	1	7	1.1	-0.7
-3	1	8	10.6	-9.1
-3	1	9	36.5	-34.4
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-3	1	11	4.5	4.9
-3	1	12	10.5	-9.9
-3	1	13	8.0	-7.3
-3	1	14	6.0	-6.3
-3	1	15	2.7	-2.3
-3	1	16	6.5	6.4
-3	1	17*	0.9	-0.2
-3	1	18	5.4	-4.8
-3	1	19	7.5	-7.4
-3	1	20*	1.0	-0.7
-3	1	21	5.8	-5.9
-3	1	22*	1.1	-1.0
-3	2	1	30.1	28.4
-3	2	2	6.8	5.2
-3	2	3	25.4	-24.1
-3	2	4	65.4	-66.0
-3	2	5*	0.6	-1.6
-3	2	6	3.9	-3.9
-3	2	7	8.9	8.2
-3	2	8	39.5	37.3
-3	2	9	1.3	-0.3
-3	2	10	48.1	-46.7
-3	2	11	8.3	-7.4
-3	2	12	6.2	-5.5
-3	2	13	7.2	-7.0
-3	2	14	23.1	22.8
-3	2	15	4.9	4.7
-3	2	16	25.0	-25.3
-3	2	17	5.2	4.1
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-3	2	21	2.2	1.2
-3	2	22	2.6	-2.3
-3	3	1	12.7	-10.7
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-3	3	3	29.8	-29.3
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-3	3	10	12.6	-11.8
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-3	3	12*	0.8	0.3
-3	3	13	7.8	-7.4
-3	3	14	5.7	-5.9
-3	3	15	10.7	-10.0
-3	3	16	18.7	19.9
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-3	3	20*	1.0	-0.8
-3	3	21*	1.1	-1.6
-3	3	22*	1.1	-1.2
-3	4	1	13.7	13.2
-3	4	2	26.1	25.5
-3	4	3	2.0	1.9
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-3	4	8	26.8	25.1
-3	4	9	11.0	-10.5
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-3	4	15	2.9	-3.0
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-3	4	17	4.2	4.1
-3	4	18	11.4	-11.3
-3	4	19	2.7	2.5
-3	4	20	6.4	6.2
-3	4	21*	1.1	-0.8
-3	5	1	42.9	-42.9
-3	5	2*	0.6	-0.2
-3	5	3	1.5	-2.2
-3	5	4	13.3	11.1
-3	5	5	50.4	49.2
-3	5	6	8.9	-9.3
-3	5	7	16.4	-15.8
-3	5	8	6.9	6.8
-3	5	9*	0.7	-0.6
-3	5	10	10.1	-9.7
-3	5	11	2.5	-3.3
-3	5	12	20.0	-19.4
-3	5	13	16.7	-16.9
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-3	5	16	8.0	7.9
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-3	5	18*	1.0	-0.7
-3	5	19	4.1	-4.0
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-3	5	21*	1.1	0.4
-3	6	1	6.2	5.7
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-3	7	19*	1.0	-0.5
-3	8	1	7.3	7.8
-3	8	2	19.2	18.2
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-3	8	6	2.1	-1.9
-3	8	7	6.8	6.7
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-3	8	12*	0.8	0.1
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-3	9	2*	0.6	0.5
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-3	10	14*	0.9	0.4
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-3	11	11*	0.8	-0.8
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-3	11	13	5.9	-6.2
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-3	12	4*	0.7	-0.9
-3	12	5	5.4	-5.3
-3	12	6	2.0	-1.8
-3	12	7	6.6	6.7
-3	12	8	7.5	7.2
-3	12	9*	0.7	0.9
-4	0	2	14.4	14.2
-4	0	4	32.6	-31.4
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-4	0	8	9.2	8.9
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-4	0	12	13.5	-12.8
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-4	1	1	37.4	-36.2
-4	1	2	19.2	18.5
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-4	1	23*	1.1	0.7
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-4	2	19*	1.0	-1.0
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-4	2	21	4.1	-3.5
-4	2	22	1.8	-2.4
-4	3	1	16.5	-15.1
-4	3	2*	0.7	0.2
-4	3	3	10.8	10.3
-4	3	4	17.5	-15.9
-4	3	5	39.5	36.2
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-4	3	20*	1.0	-0.1
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-4	3	22*	1.1	0.9
-4	4	1	8.9	-8.7
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-4	4	21*	1.1	-0.4
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-4	8	2	5.0	-4.8
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-4	11	1*	0.8	-1.4
-4	11	2	9.8	9.5
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-4	12	3*	0.6	1.1
-4	12	4	12.3	-12.0
-4	12	5*	0.8	0.1
-4	12	6	2.5	2.7
-4	12	7	5.4	-4.8
-5	0	2	4.5	4.0
-5	0	4	14.9	12.9
-5	0	6	4.3	3.2
-5	0	8	16.7	-16.0
-5	0	10	4.5	3.0
-5	0	12	32.4	31.6
-5	0	14	3.0	-3.0
-5	0	16	9.1	9.0
-5	0	18	6.4	6.5
-5	0	20	1.0	-1.2
-5	0	22	3.2	3.4
-5	1	1	23.5	22.5
-5	1	2	3.7	-3.7
-5	1	3	9.3	8.3
-5	1	4	2.2	1.9
-5	1	5	29.0	-27.6
-5	1	6	17.6	16.1
-5	1	7	23.1	21.5
-5	1	8	4.4	4.1
-5	1	9	12.4	12.0
-5	1	10*	0.8	1.2
-5	1	11	24.3	-23.6
-5	1	12	5.8	5.6
-5	1	13	17.7	17.2
-5	1	14	2.2	2.1
-5	1	15	15.6	14.9
-5	1	16	4.6	-4.1
-5	1	17	12.0	-11.7
-5	1	18*	1.0	-0.5
-5	1	19	6.1	6.1
-5	1	20	6.3	6.4
-5	1	21	9.9	9.9
-5	1	22	2.2	2.2
-5	1	23	3.9	-3.5
-5	2	1	5.5	5.4
-5	2	2	32.5	-31.2
-5	2	3	11.8	-11.8
-5	2	4	8.2	7.7
-5	2	5	11.4	11.5
-5	2	6	21.4	21.4
-5	2	7	2.6	3.2
-5	2	8	21.6	-20.9
-5	2	9	6.9	6.4
-5	2	10	7.3	-6.4
-5	2	11	4.4	-4.0
-5	2	12	18.3	18.4
-5	2	13	2.5	-3.1
-5	2	14	12.7	-12.9
-5	2	15	1.6	0.7
-5	2	16*	0.9	-0.6
-5	2	17	4.6	4.4
-5	2	18	7.9	7.9
-5	2	19	2.9	-3.0
-5	2	20	2.8	-2.5
-5	2	21	1.9	1.7
-5	2	22	1.8	1.1
-5	3	1	11.0	11.2
-5	3	2	4.0	3.4
-5	3	3	16.5	16.2
-5	3	4	9.5	-9.8
-5	3	5	22.0	-21.9
-5	3	6	14.6	-13.3
-5	3	7	10.9	10.0
-5	3	8	10.0	-10.1
-5	3	9	18.9	18.1
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-5	3	12	3.4	-3.3
-5	3	13	8.3	8.6
-5	3	14	2.6	2.5
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-5	3	17	10.9	-11.1
-5	3	18	6.9	-6.9
-5	3	19	10.4	10.6
-5	3	20	5.5	-5.8
-5	3	21	8.7	9.1
-5	3	22*	1.1	-0.6
-5	4	1	11.0	10.6
-5	4	2	12.2	-12.2
-5	4	3	10.6	10.9
-5	4	4	15.7	14.9
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-5	4	7	26.3	-25.5
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-5	4	9	10.9	-10.4
-5	4	10	8.2	8.5
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-5	4	12	5.9	5.8
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-5	4	19	12.6	-11.7
-5	4	20*	1.1	1.1
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-5	4	22	2.4	2.6
-5	5	1	9.7	9.6
-5	5	2	20.7	20.2
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-5	5	5	22.4	-22.6
-5	5	6	4.6	-4.2
-5	5	7	14.0	13.9
-5	5	8*	0.8	1.1
-5	5	9	13.4	13.7
-5	5	10	4.7	-4.4
-5	5	11	27.5	-27.1
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-5	5	19	2.4	3.2
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-5	5	21	5.4	5.9
-5	6	1	11.4	11.4
-5	6	2	12.5	-12.4
-5	6	3*	0.8	0.2
-5	6	4*	0.8	1.5
-5	6	5	6.2	-6.8
-5	6	6	11.5	11.8
-5	6	7	6.0	6.1
-5	6	8	13.9	-14.2
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-5	6	14	3.3	-3.4
-5	6	15	3.3	3.0
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-5	6	17	3.0	3.3
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-5	7	6*	0.8	1.0
-5	7	7	8.0	8.5
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-5	7	9	7.2	7.2
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-5	7	12*	0.9	-0.1
-5	7	13	7.0	7.3
-5	7	14	2.8	2.8
-5	7	15	5.3	5.4
-5	7	16	3.4	-3.3
-5	7	17	6.3	-6.6
-5	7	18*	1.0	-0.8
-5	7	19	7.7	3.1
-5	8	1	2.7	-3.0
-5	8	2	12.5	-12.9
-5	8	3*	0.8	0.4
-5	8	4	2.0	2.0
-5	8	5	2.6	-3.0
-5	8	6	18.7	18.9
-5	8	7	1.2	-0.5
-5	8	8	4.1	-4.0
-5	8	9*	0.8	1.3
-5	8	10	4.3	4.8
-5	8	11	8.1	8.0
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-5	8	15*	0.9	-0.1
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-5	8	18	8.5	8.8
-5	9	1	4.5	4.4
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-5	9	4	2.9	-3.3
-5	9	5	10.7	-10.7
-5	9	6*	0.8	-1.7
-5	9	7	13.6	14.3
-5	9	8	6.6	6.7
-5	9	9	10.5	11.2
-5	9	10*	0.8	1.2
-5	9	11	11.1	-11.3
-5	9	12*	0.9	0.8
-5	9	13	2.2	2.0
-5	9	14	6.0	5.5
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-5	10	2	3.4	-3.6
-5	10	3	2.9	2.6
-5	10	4	4.4	4.1
-5	10	5*	0.8	-0.8
-5	10	6	2.8	3.3
-5	10	7	1.3	-1.5
-5	10	8	6.0	-5.6
-5	10	9	1.4	-1.5
-5	10	10*	0.9	0.7
-5	10	11	6.8	7.1
-5	10	12	3.6	3.7
-5	10	13*	0.9	0.1
-5	10	14	4.5	-4.8
-5	11	3	2.7	2.8
-5	11	4	2.3	-2.3
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-6	1	19	5.6	5.3
-6	1	20*	1.1	-1.1
-6	1	21*	1.1	0.5
-6	1	22	3.0	-2.8
-6	2	1	1.7	-2.1
-6	2	2	15.3	-14.3
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-6	2	14*	0.9	-0.2
-6	2	15*	0.9	-0.7
-6	2	16	18.9	19.3
-6	2	17*	1.0	1.4
-6	2	18*	1.0	1.4
-6	2	19	3.5	3.8
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-6	2	21*	1.1	-2.1
-6	2	22	2.5	2.7
-6	3	1	12.1	11.8
-6	3	2*	0.9	-0.5
-6	3	3	1.9	-2.0
-6	3	4*	0.9	0.4
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-6	3	8	14.3	14.4
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-6	3	14*	0.9	-0.1
-6	3	15	5.6	5.7
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-6	3	18	3.2	3.1
-6	3	19	2.0	2.5
-6	3	20*	1.1	0.7
-6	3	21	3.0	-3.4
-6	3	22*	1.1	0.6
-6	4	1	7.7	-7.8
-6	4	2	10.3	-10.3
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-6	4	12*	0.9	0.2
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-6	4	14	7.1	-7.2
-6	4	15	6.7	6.9
-6	4	16	11.7	12.0
-6	4	17*	1.0	-1.0
-6	4	18	1.9	-2.4
-6	4	19*	1.0	0.6
-6	4	20	4.7	-4.4
-6	4	21*	1.1	1.5
-6	5	1	7.3	7.9
-6	5	2	14.7	-14.3
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-6	5	4	8.2	-8.4
-6	5	5	5.0	-4.9
-6	5	6*	0.9	-0.5
-6	5	7	12.3	12.0
-6	5	8	2.3	2.3
-6	5	9	3.7	-4.0
-6	5	10*	0.9	-0.8
-6	5	11	9.9	-9.8
-6	5	12*	0.9	1.6
-6	5	13	6.3	6.2
-6	5	14	2.8	-3.0
-6	5	15	2.3	-2.8
-6	5	16*	1.0	-0.3
-6	5	17	4.7	-4.7
-6	5	18	2.2	-2.2
-6	5	19*	1.1	1.1
-6	5	20	1.8	-2.1
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-6	6	2	17.9	-18.4
-6	6	3	8.2	-8.2
-6	6	4*	0.9	-0.4
-6	6	5	8.2	-8.0
-6	6	6	6.1	-6.0
-6	6	7	1.9	1.3
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-6	6	9	7.7	8.0
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-6	6	11*	0.9	0.1
-6	6	12*	0.9	1.2
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-6	6	14	14.7	-15.2
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-6	6	16	1.6	2.0
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-6	6	18	3.0	-3.2
-6	6	19	1.7	-1.4
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-6	7	8*	0.9	1.1
-6	7	9*	0.9	0.1
-6	7	10	5.9	6.3
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-6	7	12	4.0	3.8
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-6	7	17*	1.0	-1.0
-6	7	18	2.5	2.7
-6	8	1*	1.0	0.6
-6	8	2	6.5	-6.8
-6	8	3	2.4	3.0
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-6	8	6	4.8	-5.0
-6	8	7*	0.9	0.7
-6	8	8	5.5	-6.0
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-6	8	17*	1.0	0.7
-6	9	1	5.6	5.6
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-6	9	6	1.5	1.6
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-6	9	8	1.6	1.7
-6	9	9*	0.9	0.2
-6	9	10	1.9	2.0
-6	9	11	5.1	-5.1
-6	9	12	3.1	-3.6
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-6	9	14*	1.0	-0.4
-6	10	4	1.6	2.1
-6	10	5	6.8	-6.4
-6	10	6	3.4	-3.7
-6	10	7*	0.9	-0.2
-6	10	8	2.7	-3.0
-6	10	9	3.4	3.2
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-7	1	2*	1.0	0.2
-7	1	3	21.2	-21.4
-7	1	4	6.9	7.0
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-7	1	7*	0.9	1.1
-7	1	8	5.8	-5.9
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-7	1	11	5.8	6.0
-7	1	12*	1.0	0.5
-7	1	13	6.0	6.0
-7	1	14	4.7	4.5
-7	1	15	15.9	-16.1
-7	1	16	3.3	3.1
-7	1	17	4.3	4.5
-7	1	18	3.6	3.6
-7	1	19*	1.1	0.8
-7	1	20*	1.1	0.3
-7	1	21	6.9	-7.0
-7	2	1*	1.0	0.1
-7	2	2	8.7	8.8
-7	2	3*	1.0	-0.1
-7	2	4	7.4	-7.6
-7	2	5*	1.0	-1.3
-7	2	6	13.5	-13.7
-7	2	7*	0.9	-1.3
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-7	2	10	4.3	4.3
-7	2	11*	1.0	1.2
-7	2	12	12.8	-12.6
-7	2	13	2.2	-2.3
-7	2	14	10.0	10.0
-7	2	15*	1.0	0.8
-7	2	16	1.6	-1.0
-7	2	17*	1.0	0.5
-7	2	18	10.1	-10.0
-7	2	19*	1.1	0.5
-7	2	20	4.4	4.6
-7	2	21*	1.1	0.7
-7	3	1	1.6	-1.7
-7	3	2*	1.0	1.2
-7	3	3	14.0	-14.9
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-7	3	8	2.4	-3.0
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-7	3	11	12.7	12.5
-7	3	12	3.5	-3.6
-7	3	13	5.8	5.8
-7	3	14*	1.0	0.9
-7	3	15	15.3	-15.6
-7	3	16	4.5	-4.7
-7	3	17*	1.0	-0.5
-7	3	18	4.1	-4.5
-7	3	19	1.8	1.2
-7	3	20	2.9	-3.2
-7	3	21	6.4	-6.8
-7	4	1*	1.0	-2.1
-7	4	2	10.3	10.4
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-7	4	4	6.6	-6.6
-7	4	5	9.8	-9.8
-7	4	6	18.9	-19.8
-7	4	7*	1.0	1.3
-7	4	8	10.2	10.3
-7	4	9	4.7	4.9
-7	4	10	5.2	-5.3
-7	4	11	3.3	4.2
-7	4	12	10.6	-11.5
-7	4	13	3.8	3.5
-7	4	14	10.4	10.6
-7	4	15	2.7	-3.0
-7	4	16	6.1	-6.4
-7	4	17	11.3	-11.7
-7	4	18	11.4	-11.6
-7	4	19	4.2	-4.6
-7	4	20	2.7	2.5
-7	5	1*	1.0	-0.7
-7	5	2	1.9	-2.2
-7	5	3	8.9	-9.1
-7	5	4	6.7	-7.0
-7	5	5	5.6	6.0
-7	5	6*	1.0	0.8
-7	5	7	7.4	7.6
-7	5	8	2.5	2.4
-7	5	9	16.7	-17.7
-7	5	10	6.4	7.2
-7	5	11	1.5	-0.8
-2	5	12	4.5	5.0
-7	5	13	2.6	2.4
-7	5	14*	1.0	-0.7
-7	5	15	6.6	-6.9
-7	5	16	5.4	-5.7
-7	5	17	1.9	2.0
-7	5	18	1.6	-1.4
-7	5	19	3.1	3.4
-7	6	1*	1.0	1.5
-7	6	2	14.4	14.8
-7	6	3	2.3	-2.5
-7	6	4	4.5	4.9
-7	6	5	3.6	-3.8
-7	6	6	9.9	-10.4
-7	6	7	3.3	3.4
-7	6	8	8.4	8.8
-7	6	9	1.8	1.6
-7	6	10	4.0	-4.6
-7	6	11	1.7	1.5
-7	6	12	8.1	-8.5
-7	6	13*	1.0	-0.1
-7	6	14	9.1	9.6
-7	6	15	2.3	-2.8
-7	6	16*	1.0	0.9
-7	6	17*	1.1	-0.5
-7	6	18	4.5	-4.7
-7	7	1*	1.0	-1.4
-7	7	2	3.3	-3.4
-7	7	3	2.7	-2.9
-7	7	4	1.6	-1.3
-7	7	5	7.3	7.8
-7	7	6*	1.0	0.3
-7	7	7	2.4	3.0
-7	7	8	2.0	-1.4
-7	7	9	12.0	-12.6
-7	7	10	3.1	-3.3
-7	7	11	5.3	5.5
-7	7	12*	1.0	-0.1
-7	7	13*	1.0	-0.9
-7	7	14	3.3	-3.9
-7	7	15	6.7	-7.1
-7	7	16*	1.0	-0.2
-7	8	3	2.6	-2.7
-7	8	4	2.9	-3.0
-7	8	5	3.3	-3.0
-7	8	6	9.1	-9.2
-7	8	7*	1.0	0.9
-7	8	8	6.9	7.3
-7	8	9*	1.0	-1.7
-7	8	10	3.9	-4.2
-7	8	11	4.8	-4.8
-7	8	12	9.6	-10.2
-7	8	13*	1.0	-0.1
-7	8	14	4.2	4.5
-8	0	2*	1.1	1.4
-8	0	4*	1.1	1.5
-8	0	6	5.0	5.3
-8	0	8	5.3	5.9
-8	0	10	1.7	-2.2
-8	0	12	12.3	11.4
-8	0	14	5.4	5.8
-8	0	16	5.2	-4.8
-8	0	18*	1.1	-1.1
-8	0	20	4.6	4.4
-8	1	1	4.7	-5.4
-8	1	2*	1.1	-1.1
-8	1	3	4.0	4.8
-8	1	4*	1.1	-0.1
-8	1	5	8.0	8.4
-8	1	6*	1.0	-0.3
-8	1	7	5.3	-5.9
-8	1	8*	1.0	-0.9
-8	1	9*	1.0	1.5
-8	1	10*	1.0	-0.3
-8	1	11	9.5	9.8
-8	1	12	3.4	3.6
-8	1	13	2.7	-3.1
-8	1	14*	1.0	1.7
-8	1	15	3.7	3.7
-8	1	16*	1.1	0.3
-8	1	17	1.7	1.3
-8	1	18	3.9	-3.6
-8	1	19	6.6	-6.7
-8	1	20	3.2	-2.7
-8	2	1	3.7	3.5
-8	2	2*	1.1	-0.1
-8	2	3	2.4	-2.2
-8	2	4	4.8	-5.0
-8	2	5*	1.1	-0.7
-8	2	6	1.0	0.2
-8	2	7	2.9	-2.5
-8	2	8	4.1	4.1
-8	2	9*	1.0	-0.1
-8	2	10	3.0	-3.2
-8	2	11	1.9	1.5
-8	2	12	3.1	3.3
-8	2	13	2.5	2.9
-8	2	14	3.2	3.5
-8	2	15	1.8	-2.3
-8	2	16	4.2	-4.5
-8	2	17*	1.1	0.1
-8	2	18	7.5	-7.7
-8	2	19	3.1	-3.2
-8	3	1	4.4	-5.1
-8	3	2*	1.1	0.7
-8	3	3	2.0	2.3
-8	3	4	2.3	2.4
-8	3	5	6.5	6.9
-8	3	6	1.7	2.3
-8	3	7	7.9	-8.4
-8	3	8	3.1	3.5
-8	3	9	2.6	3.2
-8	3	10	3.8	-5.1
-8	3	11	11.1	11.7
-8	3	12	4.6	-5.3
-8	3	13	2.8	-3.2
-8	3	14	1.9	-2.0
-8	3	15*	1.1	0.8
-8	3	16	2.7	2.9
-8	3	17*	1.1	-0.8
-8	3	18*	1.1	-0.2
-8	3	19	7.3	-8.5
-8	4	1*	1.1	-0.3
-8	4	2	1.7	1.9
-8	4	3*	1.1	-0.8
-8	4	4*	1.1	-1.6
-8	4	5	9.4	9.5
-8	4	6	8.1	8.3
-8	4	7	5.7	5.9
-8	4	8	3.6	3.9
-8	4	9	3.9	-4.2
-8	4	10*	1.0	1.1
-8	4	11	9.0	-9.7
-8	4	12	5.3	5.8
-8	4	13*	1.1	-0.9
-8	4	14	5.0	5.1
-8	4	15*	1.1	-0.7
-8	4	16	2.9	-2.7
-8	4	17	2.1	2.2
-8	4	18*	1.1	-0.7
-8	5	2*	1.1	-0.1
-8	5	3	1.8	-1.7
-8	5	4	4.8	5.7
-8	5	5	8.0	8.8
-8	5	6	4.2	4.8
-8	5	7	1.6	-1.3
-8	5	8	3.7	3.8
-8	5	9	5.4	5.7
-8	5	10	2.8	-3.5
-8	5	11	4.8	5.9
-8	5	12	7.5	-7.9
-8	5	13	6.4	-6.6
-8	5	14	2.0	-2.4
-8	5	15*	1.1	0.1
-8	5	16	2.7	2.6
-8	5	17	5.3	5.4
-8	6	5	2.8	3.3
-8	6	6	4.2	4.8
-8	6	7*	1.1	0.7
-8	6	8*	1.1	-0.3
-8	6	9*	1.1	-0.8
-8	6	10	2.5	-2.7
-8	6	11*	1.1	-1.5
-8	6	12	2.9	-2.8
-8	6	13	2.4	-2.5
-8	6	14*	1.1	0.8
-8	6	15	2.9	-2.7
-9	0	6	9.0	9.9
-9	0	8	5.5	-5.3
-9	0	10	4.6	-4.5
-9	0	12	9.7	10.4
-9	0	14*	1.1	1.0
-9	0	16	6.9	-6.8
-9	1	6	2.2	0.1
-9	1	7*	1.1	1.1
-9	1	8*	1.1	0.8
-9	1	9	8.4	8.5
-9	1	10*	1.1	-1.1
-9	1	11	3.8	-3.7
-9	1	12	2.5	-3.0
-9	1	13	3.1	-3.1
-9	1	14*	1.1	-1.6
-9	1	15	6.9	7.0
-9	1	16*	1.1	-1.0
-9	2	7*	1.1	1.1
-9	2	8	3.8	4.1
-9	2	9*	1.1	1.1
-9	2	10	3.1	-3.5
-9	2	11*	1.1	1.1
-9	2	12	4.6	4.9
-9	2	13	3.4	-3.2
-9	2	14*	1.1	-1.8
-9	2	15*	1.1	-0.7
-9	3	8	4.2	4.2
-9	3	9	9.0	9.8
-9	3	10*	1.1	2.3
-9	3	11	3.9	-4.5
-9	3	12*	1.1	0.5
-9	3	13	3.3	-4.0
-9	3	14*	1.1	-0.8

Crystal data

Adrenalone, 2-methylamino-1-(3,4-dihydroxyphenyl) ethane-1-one hydrochloride monohydrate,
$C_9H_{11}O_3N.HCl.H_2O$.
$a = 7·133$ Å   M.W. = 235·67
$b = 10·138$ $V = 1113·63$ Å^3
$c = 17·614$ $D_m = 1·399$ g.cm^{-3}
$\beta = 119·04°$ $D_x(Z=4) = 1·405$ g.cm^{-3}.
Absent spectra, $0k0$ when k is odd, $h0l$ when l is odd.
Space group $P2_1/c$.

When recalculating unit-cell dimensions to the cell adopted by Faber (1929) one obtains $a:b:c = 1·5254:1:0·7036$, $\beta = 95·26°$ which are in good agreement with the values $a:b:c = 1·5251:1:0·7047$, $\beta = 95·19°$ (mean values) given by Faber (1930).

Intensities within a quarter-sphere ($\sin\theta/\lambda = 0·65$), corresponding to that of Cu $K\alpha$, were collected with strictly monochromatic Mo $K\alpha$ radiation in an automatic linear diffractometer (PAILRED). Depending on the intensities, the reflexions were scanned from 1 to 7 times, thereby approaching fixed-count strategy. The background was counted for two minutes on each side of every reflexion. In all, 2801 independent reflexions were recorded. Apart from 150 systematic absences, 380 reflexions did not differ significantly from the background. These unobserved reflexions were given half the threshold intensity when included in the calculations. Reflexions were corrected for background and for Lorentz and polarization factors, but not for extinction or absorption; subsequently the structure factors were placed approximately on an absolute scale by Wilson statistics. The above calculations were performed with program system *CRYSTAL* (Bergin & Ringertz, 1969) on an IBM 360/75 computer. This computer was also used for the final thermal-ellipsoid drawing utilizing program *ORTEP* (Johnson, 1965). All other computations were made with the *X-RAY*-63 system (Stewart & High, 1965) on an IBM 7090 computer.

Structure determination and refinement

The chlorine atom was easily located using three-dimensional Patterson synthesis. In graphical three-dimensional minimum functions according to Buerger (1959), 13 distinct maxima were obtained. The minimum functions were derived from Cl–Cl inversion peaks as well as rotation peaks. The latter could be used in this case as the y coordinate for Cl was found to be $\simeq 0$ or $\frac{1}{2}$. Although it was not possible to locate the adrenalone molecules in these maps it was felt they were essentially correct. Besides the chlorine peak six other prominent maxima were selected, and in a three-dimensional electron-density synthesis phased upon the positions of these seven atoms, the remaining non-hydrogen atoms were easily identified. A structure-factor calculation with positional coordinates from the electron-density maps and with an overall B value of 3·0 Å^2 gave an R value of 24% $[R = \sum(|F_o| - |F_c|)/\sum|F_o|]$.

The structure was refined using the full-matrix least-squares method and atomic scattering factors from *International Tables for X-ray Crystallography* (1962). Because of the counter strategy, structure amplitudes were given unit weight. Two cycles of refinement with observed structure amplitudes only and $B = 3·0$ Å^2 brought the R value down to 12·1%, and two further cycles with individual isotropic thermal parameters reduced R to 7·6%. A difference electron-density map at this stage showed unequivocally positions of the 14 hydrogen atoms that in subsequent refinements were given a temperature factor of $B = 3·0$ Å^2. With the hydrogen atoms introduced, and anisotropic thermal parameters for the non-hydrogen atoms, the R value dropped to 4·8% after four cycles of further refinement. The average shift-to-error ratio in the last cycle for the 178 parameters that were varied was 0·65, and the final R value for all reflexions was 5·4%. Final observed and calculated structure factors are listed in Table 1. Positional and thermal parameters for the final structure are given in Tables 2 and 3, respectively.

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

	x/a	y/b	z/c
Cl	0·22585 (10)	0·00535 (7)	0·33612 (4)
O(1)	0·8667 (3)	0·2875 (2)	0·6578 (1)
O(2)	0·9677 (3)	0·5333 (2)	0·6347 (1)
O(3)	0·5623 (3)	0·6161 (2)	0·3132 (1)
O(4)	0·0537 (4)	0·6957 (2)	0·1210 (2)
N	0·3423 (3)	0·4911 (2)	0·1652 (1)
C(1)	0·5463 (4)	0·3151 (2)	0·4207 (2)
C(2)	0·6319 (4)	0·2602 (2)	0·5030 (2)
C(3)	0·7737 (4)	0·3319 (2)	0·5745 (2)
C(4)	0·8294 (4)	0·4598 (2)	0·5642 (2)
C(5)	0·7457 (4)	0·5146 (2)	0·4831 (2)
C(6)	0·6030 (4)	0·4427 (2)	0·4101 (1)
C(7)	0·5214 (4)	0·5039 (2)	0·3240 (2)
C(8)	0·3798 (4)	0·4207 (3)	0·2448 (2)
C(9)	0·2236 (5)	0·4094 (3)	0·0854 (2)
H(1)	0·452 (5)	0·271 (3)	0·376 (2)
H(2)	0·586 (5)	0·166 (3)	0·510 (2)
H(3)	0·828 (5)	0·210 (3)	0·659 (2)
H(4)	1·011 (5)	0·494 (3)	0·676 (2)
H(5)	0·795 (5)	0·602 (3)	0·479 (2)
H(6)	0·435 (5)	0·331 (3)	0·243 (2)
H(7)	0·234 (5)	0·401 (3)	0·239 (2)
H(8)	0·478 (5)	0·513 (3)	0·175 (2)
H(9)	0·269 (5)	0·572 (3)	0·160 (2)
H(10)	0·295 (5)	0·329 (3)	0·093 (2)
H(11)	0·216 (5)	0·469 (3)	0·033 (2)
H(12)	0·068 (5)	0·396 (3)	0·072 (2)
H(13)	0·045 (5)	0·777 (3)	0·133 (2)
H(14)	−0·018 (5)	0·653 (3)	0·138 (2)

Description and discussion of the structure

Molecule configuration

The numbering of the atoms is given in Fig. 1 which also illustrates the configuration of the adrenalone molecule. Like other catecholamines (Carlström & Bergin, 1967; Bergin & Carlström, 1968), phenethylamine (Tsoucaris, 1961) and related derivatives such as ephedrine (Phillips, 1954; Bergin, 1971), pseudoephedrine (Bailey, Harrison & Mason, 1968) and amphetamine (Bergin & Carlström, 1971), the adrenalone molecule is maximally extended, *i.e.* the amino nitrogen is as far as possible from the six-membered ring. The planarity of this ring is excellent, the maximal

Table 3. *Anisotropic thermal parameters and their standard deviations in parentheses*

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

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cl	0·0207 (2)	0·0075 (1)	0·0038 (0)	−0·0001 (1)	0·0036 (1)	0·0005 (0)
O(1)	0·0350 (6)	0·0084 (2)	0·0034 (1)	−0·0041 (3)	0·0044 (2)	0·0005 (1)
O(2)	0·0292 (6)	0·0073 (2)	0·0031 (1)	−0·0036 (3)	0·0017 (2)	0·0000 (1)
O(3)	0·0354 (7)	0·0059 (2)	0·0035 (1)	−0·0031 (3)	0·0031 (2)	0·0000 (1)
O(4)	0·0341 (7)	0·0077 (2)	0·0076 (1)	0·0035 (3)	0·0093 (3)	0·0013 (1)
N	0·0181 (5)	0·0066 (2)	0·0030 (1)	0·0007 (3)	0·0024 (2)	−0·0001 (1)
C(1)	0·0202 (6)	0·0058 (2)	0·0035 (1)	−0·0016 (3)	0·0042 (2)	−0·0007 (1)
C(2)	0·0246 (7)	0·0058 (2)	0·0037 (1)	−0·0020 (3)	0·0052 (3)	−0·0002 (1)
C(3)	0·0200 (6)	0·0066 (2)	0·0033 (1)	−0·0000 (3)	0·0044 (2)	0·0002 (1)
C(4)	0·0172 (6)	0·0060 (2)	0·0032 (1)	−0·0006 (3)	0·0032 (2)	−0·0004 (1)
C(5)	0·0178 (6)	0·0056 (2)	0·0033 (1)	−0·0008 (3)	0·0035 (2)	−0·0001 (1)
C(6)	0·0169 (6)	0·0054 (2)	0·0031 (1)	0·0003 (3)	0·0036 (2)	−0·0002 (1)
C(7)	0·0176 (6)	0·0058 (2)	0·0031 (1)	0·0003 (3)	0·0031 (2)	−0·0004 (1)
C(8)	0·0223 (7)	0·0066 (2)	0·0031 (1)	−0·0015 (3)	0·0029 (2)	−0·0003 (1)
C(9)	0·0266 (8)	0·0089 (3)	0·0032 (1)	0·0000 (4)	0·0013 (2)	−0·0008 (2)

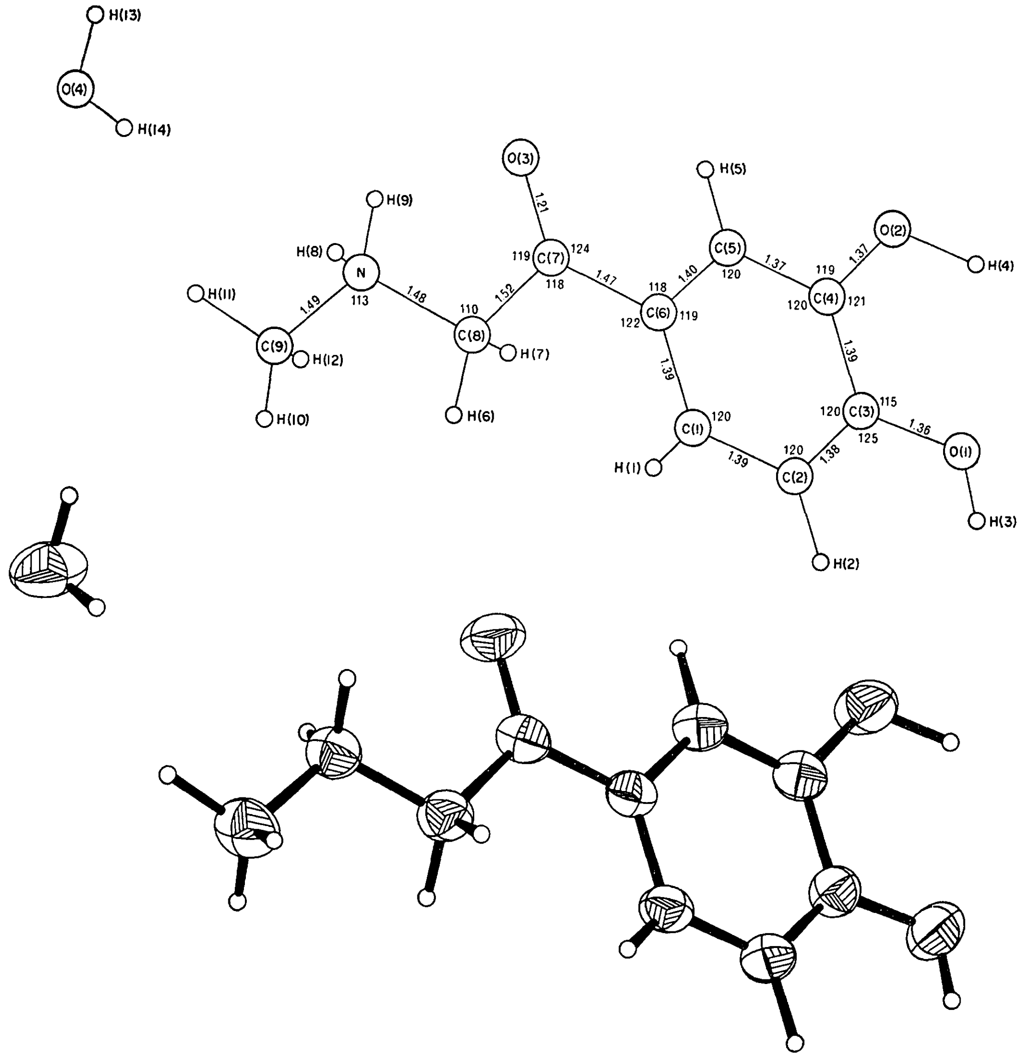

Fig. 1. Nomenclature and molecular dimensions of adrenalone. Thermal ellipsoids are at 50%-probability level. Projection is along **a***.

deviation from the best plane being only 0·004 Å (Table 4). The two oxygen atoms O(1) and O(2) are also nearly in the plane of the ring, whereas C(7) deviates significantly. As could be expected the grouping around C(7) involving the carbonyl oxygen is planar; the maximal deviation from the plane defined by C(6), C(7), C(8) and O(3) is 0·002 Å. The non-hydrogen atoms of the side chain, including C(6)–C(9), N and O(3), also form a plane but with less planarity; the largest deviation is 0·122 Å. The acute angle between this plane and that of the benzene ring is 8·2°; thus, the molecule is approximately planar. This is a conformation quite different from that of the closely related compounds cited above. In all these substances the plane of the side chain and that of the ring are near-perpendicular to each other.

Table 4. *Least-squares planes and deviations of individual atoms from these planes*

Planes are expressed as $PX+QY+RZ=S$, where X, Y, Z are orthogonal Ångström space coordinates referred to crystallographic a, b and c^* axes.

Plane of benzene ring, C(1)–C(6)

P =	−0·9271	C(1)	−0·0010 Å	C(5)	−0·0005 Å
Q =	0·3633	C(2)	−0·0020	C(6)	0·0023
R =	0·0918	C(3)	0·0038	O(1)	0·0044
S =	1·4761	C(4)	−0·0025	O(2)	−0·0166
				C(7)	0·0423

Plane of C(6)–C(8) and O(3)

P =	−0·9458	C(6)	0·0007 Å
Q =	0·3224	C(7)	−0·0022
R =	0·0382	C(8)	0·0006
S =	0·9373	O(3)	0·0009

Plane of side chain C(6)–C(9), O(3) and N

P =	−0·9516	C(6)	0·0733 Å	C(9)	0·0604 Å
Q =	0·3052	C(7)	−0·0171	O(3)	−0·0047
R =	−0·0364	C(8)	−0·1216	N	0·0096
S =	0·4570				

Bond lengths and bond angles calculated from the coordinates of Table 2 are given in Tables 5 and 6 respectively. The phenyl ring is only slightly distorted with C–C distances varying from 1·370 to 1·394 Å (average 1·387 Å). The difference in bond length between this average and the C(2)–C(3) distance is probably significant, and that of C(4)–C(5) is highly significant according to the criteria of Cruickshank (1966). This is not surprising, as it is known that different substituent groups on the benzene ring may cause slightly different C–C distances around the ring (Klug, 1970). The C(6)–C(7) separation (1·474 Å) is normal for this type of single bond, and the C–O bond (1·212 Å) agrees well with known ketonic C=O distances (Sutton, 1965). The C–N bonds (1·478 and 1·490 Å) are both slightly longer than the standard C–N bond length, but they agree well with a C–N$^+$ bond.

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

C(1)–C(2)	1·387 (4) Å	C(1)–H(1)	0·87 (3) Å
C(2)–C(3)	1·379 (3)	C(2)–H(2)	1·04 (4)
C(3)–O(1)	1·360 (3)	O(1)–H(3)	0·83 (4)
C(3)–C(4)	1·394 (4)	O(2)–H(4)	0·76 (3)
C(4)–O(2)	1·371 (3)	C(5)–H(5)	0·97 (4)
C(4)–C(5)	1·370 (3)	C(8)–H(6)	1·00 (4)
C(5)–C(6)	1·397 (3)	C(8)–H(7)	1·01 (4)
C(6)–C(1)	1·394 (4)	N—H(8)	0·92 (4)
C(6)–C(7)	1·474 (4)	N—H(9)	0·95 (4)
C(7)–O(3)	1·212 (3)	C(9)–H(10)	0·94 (3)
C(7)–C(8)	1·519 (3)	C(9)–H(11)	1·09 (4)
C(8)–N	1·478 (4)	C(9)–H(12)	1·02 (4)
N—C(9)	1·490 (3)	O(4)–H(13)	0·86 (4)
		O(4)–H(14)	0·82 (4)

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

C(6)–C(1)–C(2)	120·2 (2)°	C(3)—O(1)–H(3)	110 (2)°
C(1)–C(2)–C(3)	119·9 (2)	C(4)—O(2)–H(4)	112 (2)
C(2)–C(3)–C(4)	120·0 (2)	C(4)—C(5)–H(5)	117 (2)
C(2)–C(3)–O(1)	124·7 (2)	C(6)—C(5)–H(5)	123 (2)
C(4)–C(3)–O(1)	115·3 (2)	C(7)—C(8)–H(6)	116 (2)
C(3)–C(4)–C(5)	120·4 (2)	N—C(8)–H(6)	107 (2)
C(3)–C(4)–O(2)	120·9 (2)	C(7)—C(8)–H(7)	114 (2)
C(5)–C(4)–O(2)	118·8 (2)	N—C(8)–H(7)	107 (2)
C(4)–C(5)–C(6)	120·1 (2)	H(6)—C(8)–H(7)	103 (3)
C(5)–C(6)–C(1)	119·4 (2)	C(8)—N—H(8)	105 (2)
C(5)–C(6)–C(7)	118·4 (2)	C(9)—N—H(8)	112 (2)
C(1)–C(6)–C(7)	122·2 (2)	C(8)—N—H(9)	110 (2)
C(6)–C(7)–C(8)	117·8 (2)	C(9)—N—H(9)	111 (2)
C(6)–C(7)–O(3)	123·5 (2)	H(8)—N—H(9)	107 (3)
C(8)–C(7)–O(3)	118·7 (2)	N—C(9)–H(10)	110 (2)
C(7)–C(8)–N	109·7 (2)	N—C(9)–H(11)	105 (2)
C(8)–N—C(9)	112·7 (2)	N—C(9)–H(12)	111 (2)
C(6)–C(1)–H(1)	120 (2)	H(10)–C(9)–H(11)	114 (3)
C(2)–C(1)–H(1)	120 (2)	H(11)–C(9)–H(12)	106 (3)
C(1)–C(2)–H(2)	120 (2)	H(12)–C(9)–H(10)	112 (3)
C(3)–C(2)–H(2)	120 (2)	H(13)–O(4)–H(14)	107 (4)

As commonly found in X-ray analysis, the bonds to hydrogen atoms are roughly 0·1 Å shorter than the true internuclear distances. The eight C–H separations range from 0·87 to 1·09 Å (average 0·99 Å) and the two N–H distances are 0·92 and 0·95 Å. The four O–H distances vary from 0·76 to 0·86 Å with the average 0·82 Å, which is a trifle on the short side of the standard value. Angles involving hydrogen atoms are all quite normal.

Thermal ellipsoids drawn at the 50%-probability level are plotted in Fig. 1. While carbon atoms C(1)–C(8) have a low and slight anisotropic thermal motion, oxygen atoms O(1)–O(3) and the methyl carbon exhibit a more pronounced anisotropy and larger thermal movements with the largest component of motion approximately normal to the plane of the molecule.

Hydrogen bonds and packing of molecules

The arrangement of the molecules is shown in Fig. 2 which is an a-axis projection. As is the case in catechol (Brown, 1966) or in other catecholamines (Carlström & Bergin, 1967; Bergin & Carlström, 1968), there seem to be no intramolecular hydrogen bonds. Although the O(1)···O(2) distance (2·68 Å) is quite favourable, none of the hydrogen atoms is in a position suitable for a hydrogen-bond formation. Instead, H(3) and H(4) point towards neighbouring chlorine ions. Another intramolecular distance indicative of a hydrogen bond is N···O(3), 2·63 Å. However, in this case, the hydrogen atoms involved also point in unfavourable directions and distances H(8)···O(3) and H(9)···O(3) are too long (2·44 and 2·53 Å respectively). The structure is firmly held together by a network of hydrogen bonds shown in Fig. 2. Thus, all hydrogen atoms on N and O are involved, and the water molecule plays an important role in the hydrogen-bonding system. Distances and angles of interest are given in Table 7. Hydrogen atoms in the six hydrogen bonds lie almost in line with the donor and acceptor atoms. The four H···Cl distances vary from 2·2 to 2·5 Å and the two H···O distances are 1·8 and 2·0 Å. All other intramolecular distances agree with ordinary packing requirements.

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Table 7. *Hydrogen-bonded interactions* X–H···Y'

Columns labelled x', y', z' give the symmetry code of the acceptor atom Y'.
Reference molecule in x, y, z.

X	H	Y'	x'	y'	z'	$X\cdots Y'$	H$\cdots Y'$	X–H$\cdots Y'$
O(1)	H(3)	Cl	$\bar{x}+1$	$\bar{y}$	$\bar{z}+1$	3·054 Å	2·2 Å	171°
O(2)	H(4)	Cl	$x+1$	$\bar{y}+\frac{1}{2}$	$z+\frac{1}{2}$	3·129	2·5	147
O(4)	H(13)	O(2)	$x-1$	$\bar{y}+\frac{1}{2}$	$z-\frac{1}{2}$	2·850	2·0	168
O(4)	H(14)	Cl	$\bar{x}$	$y+\frac{1}{2}$	$\bar{z}+\frac{1}{2}$	3·119	2·3	169
N	H(9)	O(4)	x	y	z	2·756	1·8	161
N	H(8)	Cl	$\bar{x}+1$	$y+\frac{1}{2}$	$\bar{z}+\frac{1}{2}$	3·095	2·2	159

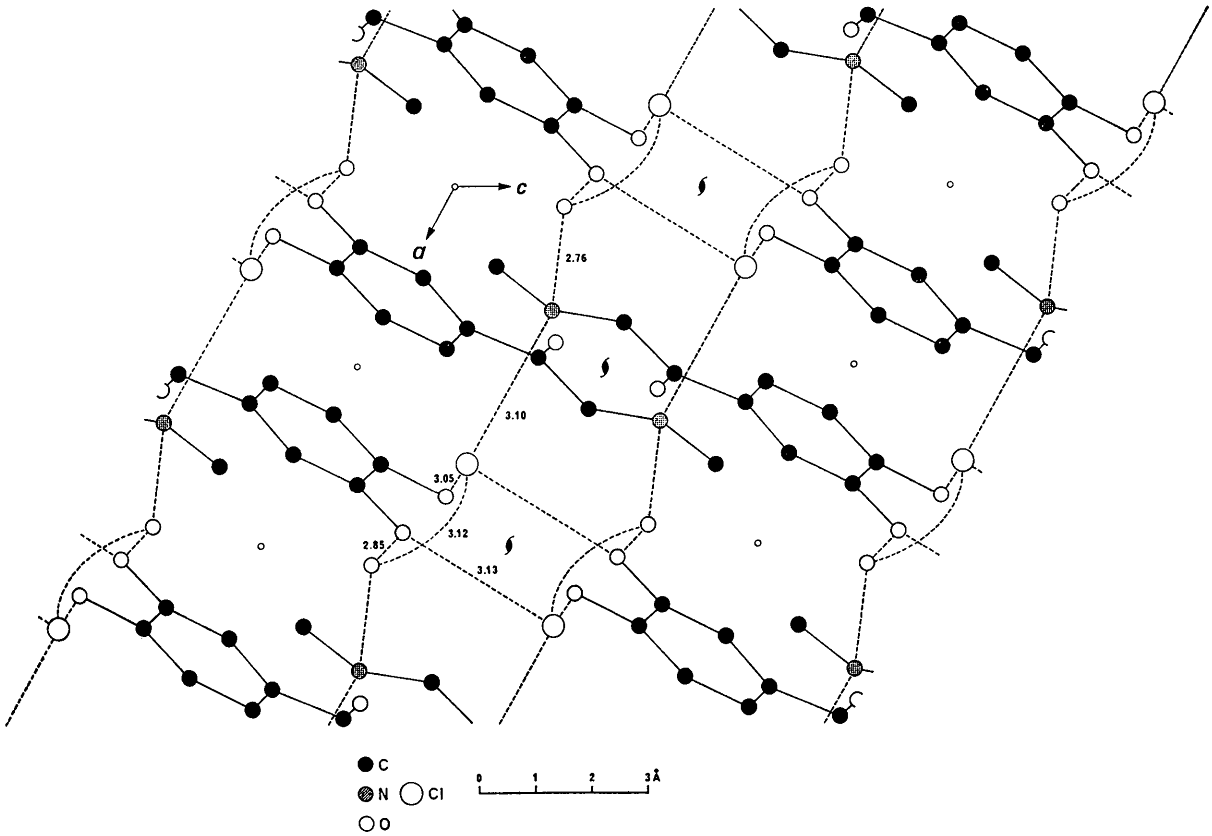

Fig. 2. Projection of adrenalone hydrochloride monohydrate structure on the (100) plane. Dashed lines indicate hydrogen bonds.

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The Crystal and Molecular Structure of Amphetamine Sulphate

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The crystals of (+)amphetamine sulphate, $(C_9H_{13}N)_2.H_2SO_4$, are monoclinic, space group $P2_1$, four formula units in a cell with $a=10{\cdot}51$, $b=6{\cdot}35$, $c=31{\cdot}34$ Å, $\beta=95{\cdot}0°$. The structure was determined by iterated Fourier synthesis and was refined by least-squares methods to an R value of 0·085 with 2917 observed reflexions. The molecules have the configuration characteristic of phenethylamine derivatives, and the structure is a layer structure with NH···O hydrogen bonds in planes parallel to {001}. Like many other layer structures the crystals exhibited stacking faults. The disorder consisted of $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ displacement of layers randomly distributed throughout the crystals.

Introduction

The basic skeleton of amphetamine is a β-phenethylamine arrangement characteristic of sympathomimetic amines, *e.g.* the neurotransmitter noradrenaline and other biologically active catecholamines. Biochemically, (+)-amphetamine releases catecholamines from their neuronal storage sites, and it has a variety of pharmacological effects. For more than 30 years it has been know as a potent stimulatory drug for the central nervous system; on chronic administration it may lead to acute paranoid psychosis.

The conformation of molecules with neurotropic activity has recently attracted considerable interest, and the present structure determination is part of our research program on biologically-active phenethylamine derivatives.

Experimental

Reagent pure (+)-amphetamine sulphate was recrystallized by evaporation of an aqueous solution. Initially prepared crystals were extremely thin plates on (001), measuring only a few μm in thickness. Crystals having dimensions suitable for single-crystal work were finally obtained after a month of extremely slow evaporation at room temperature. Considerable difficulty was experienced in selecting and trimming crystals of this batch. Weissenberg diagrams showed that most crystals were twins with the twin plane {001}. The single crystals encountered gave diagrams with pronounced streaks along $\mathbf{c}^*$ of hkl reflexions with $h+k=2n+1$. Since the crystals were easily deformable and had an eminent cleavage {001}, it was not possible to trim them mechanically. Finally, a large crystal several cm² in size with a thickness of 0·3 mm was selected, and by partial dissolution of the crystal a roughly spherical piece measuring 0·28 × 0·31 × 0·35 mm was produced. Although this crystal also gave faint streaks of the aforementioned reflexions in Weissenberg diagrams, it was the best that could be obtained for intensity measurements.

Unit-cell dimensions were determined in a linear automatic diffractometer. Density was measured by flotation in an xylene–chloroform mixture.