The Crystal and Molecular Structure of Tyramine Hydrochloride

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The structure of tyramine hydrochloride has been determined by X-ray diffraction method using the data collected by counter diffractometer techniques. Crystals are orthorhombic, with space group *Pbcn*, $Z=8$, $a=19.961$, $b=10.756$, and $c=8.243$ Å. The structure was solved by the direct method with the symbolic addition procedure, and refined by least-squares method. The atoms constituting the tyramine cation lie on the two planes, that is, that of the phenol ring and that of the extended side chain. The dihedral angle between these two planes is 71°. The extended conformation about the C–C bond of aminoethyl group is such that the NH_3^+ group is *trans* with respect to the phenol ring. Half-weighted two independent chlorine ions are found on the two-fold axis with distance of 4.5 Å, having some different modes of hydrogen-bonding system for these two ions.

Tyramine, the decarboxylated amine of tyrosine, is a precursor of *p*-hydroxyphenylacetate in the metabolic pathway of L-tyrosine. It is of particular interest to investigate systematically the structure-activity relationship among tyrosine metabolites, in view of some very important findings about the correlation between the molecular structures and metabolic pathway of tryptophan which were already reported by us.[1-4] This work is undertaken as a part of the programme of studying the crystal structures of the aromatic amino acid metabolites.

Experimental

Commercially obtained tyramine hydrochloride was dissolved in methanol. By slow evaporation, very thin colorless plate-like crystals were grown at room temperature. Oscillation and Weissenberg photographs around the *b*- and *c*-axes showed the crystal to be orthorhombic. From the systematic extinctions, the space group was uniquely determined as *Pbcn*. Unit cell parameters were determined with a Rigaku Denki four circle diffractometer. Density was measured by the flotation method in a mixture of benzene and carbon tetrachloride. The crystal data are listed in Table 1. Three-

Table 1. Crystal data of tyramine hydrochloride

$C_8H_{11}NO\cdot HCl$, M.W. 173.64
colorless and transparent plates, Orthorhombic
$a=19.961(14)$, $b=10.756(7)$, $c=8.243(3)$ Å
$V=1769.8$ Å^3, $Z=8$, $F(000)=736$
μ(for Cu$K\alpha$) $=33.7$ cm^{-1}
$D_m=1.301$ g/cm^3, $D_x=1.303$ g/cm^3
Absent spectra; $(0kl)$: $k=2n+1$
$(h0l)$: $l=2n+1$
$(hk0)$: $h+k=2n+1$
Space group; *Pbcn*

dimensional intensity data were recorded on a computer-controlled four circle diffractometer with Ni-filtered Cu-$K\alpha$ radiation using a crystal mounted about the *b*-axis. The ω-2θ scanning mode was employed at a rate of 2° per minute through the scanning range of $2\theta-0.6°$ for $K\alpha_1$ and $2\theta+0.6°$ for $K\alpha_2$. Background countings were taken for 10 seconds at both sides of each peak. In order to correct the intensities for coincidence loss, the counting rate was kept less than 8000 counts per second with an automatic attenuator mechanism. The intensities of three standard reflections measured for every 25 reflections of the data set showed no decrease in intensity during the run.

The intensities were measured for the 1168 independent reflections with $\sin\theta/\lambda$ less than 0.54. Of these, 576 had the net intensity exceeded three times of its estimated standard deviation; the rest was regarded as unobserved reflections. The data were then adjusted to the absolute scale and normalized structure factor, E, and a list of $\sum_2$ relationships with proper probabilities were calculated.

Determination and Refinement of Structure

The structure of tyramine hydrochloride was solved by direct phase determination using the symbolic addition procedure.[5] Reflections with $|E|>1.2$ were selected, five of them being given a sign or a letter symbol as follows;

h	k	l	phase	$\|E\|$
1	10	1	+	3.035
13	5	2	+	3.185
15	5	1	+	2.567
18	2	2	A	2.989
15	7	2	B	3.140

The phases of 137 reflections were determined in terms of starting signs and letters, and three-dimensional E-maps were computed for the possible four cases. Of these E-maps, one (A=−, B=+) clearly revealed two independent high peaks corresponding to two chlorine atoms, with a distance of 4.5 Å lying on the two-fold axis. Furthermore, the benzene ring plane enables us to distinguish the peaks of tyramine cation from other spurious ones on this map. The positional coordinates of the twelve atoms as selected from the E-map were refined by successive Fourier syntheses.

Further refinement was carried out by the full-matrix least-squares method with unit weight. Four cycles of refinement with the isotropic temperature factor reduced an R index ($R=\sum||F_o|-|F_c||/\sum|F_o|$) to 0.157. More five cycles with anisotropic temperature factors for all non-hydrogen atoms decreased an R value to 0.129. At this stage, a difference Fourier synthesis was calculated to determine the locations of hydrogen atoms. Nine of twelve hydrogen atoms were satisfactorily located with reasonable peak heights. However, three peaks corresponding to ammonium hydrogen atoms were obscure. The positional parameters of these hydrogen atoms were estimated as follows. The amino nitrogen atom has three chlorine neighbors at reasonable

TABLE 2. OBSERVED AND CALCULATED STRUCTURE FACTORS FOR TYRAMINE HYDROCHLORIDE

The columns in each group headed by the values of h and l give k, $2|F_o|$, and $2|F_c|$.

K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC
H,L= 0 0			2	84	-90	2	27	31	H,L= 13 2			1	32	31	1	25	17	0	39	21
2	75	-71	4	78	84	H,L= 19 1			0	23	-12	2	31	-32	5	33	-43	4	43	45
4	75	66	6	30	-30	1	24	28	1	24	-26	3	69	-81	6	23	-14	5	22	24
8	41	49	8	104	-101	3	35	32	2	35	45	6	30	25	H,L= 16 4			7	62	74
H,L= 1 0			10	40	-33	H,L= 20 1			3	30	30	H,L= 15 3			1	28	24	H,L= 4 6		
1	41	36	H,L= 1 1			2	34	40	4	51	57	1	26	-27	2	32	37	0	75	-64
3	115	-101	1	39	-37	H,L= 0 2			5	116	119	3	26	-25	5	25	1	2	60	-54
5	169	-157	2	296	306	0	156	141	6	25	-20	4	26	33	H,L= 17 4			4	37	-32
7	47	-41	3	41	36	2	375	-411	7	33	-17	H,L= 16 3			3	23	-17	H,L= 5 6		
9	103	-100	4	43	-42	6	65	-61	H,L= 14 2			2	43	-44	H,L= 18 4			3	56	52
11	24	-14	5	108	102	8	34	35	0	91	-95	H,L= 17 3			0	82	73	4	44	-48
H,L= 2 0			7	44	-41	10	22	-23	4	25	-20	2	48	-60	1	24	-14	5	40	46
0	43	53	9	51	-51	H,L= 1 2			H,L= 15 2			3	29	-34	3	31	20	6	29	27
2	68	65	10	65	66	0	209	207	0	29	-29	4	34	32	H,L= 19 4			H,L= 6 6		
6	57	50	H,L= 2 1			1	82	-92	3	30	17	H,L= 19 3			1	23	22	0	66	-65
10	80	73	2	74	77	2	76	80	5	26	19	3	25	-16	H,L= 0 5			2	31	-28
H,L= 3 0			4	160	147	3	147	170	7	47	52	H,L= 0 4			2	101	99	6	29	-23
1	65	-64	6	37	38	5	82	86	H,L= 16 2			0	204	188	4	35	43	H,L= 7 6		
3	144	-124	7	26	26	6	34	33	0	97	-97	2	35	-31	H,L= 1 5			3	30	36
5	249	-218	8	34	-30	7	100	106	3	52	-59	4	65	66	1	78	71	4	28	17
7	54	-52	9	33	29	9	22	33	7	39	22	6	51	-56	3	41	45	5	26	44
9	42	-31	10	23	-23	10	37	-41	H,L= 17 2			8	38	44	8	23	-30	H,L= 8 6		
H,L= 4 0			11	40	-35	11	24	11	0	42	49	10	58	70	H,L= 2 5			0	106	-97
0	174	172	H,L= 3 1			H,L= 2 2			5	34	31	H,L= 1 4			1	29	-17	2	29	-33
2	256	242	1	90	88	0	324	-319	H,L= 18 2			0	59	-49	2	37	39	H,L= 9 6		
4	97	84	2	36	38	1	130	141	2	56	-64	1	71	-67	6	30	-33	0	32	-34
10	58	54	3	185	174	2	99	-118	H,L= 21 2			5	90	-104	8	32	-18	1	25	-21
H,L= 5 0			4	102	-94	3	69	-74	0	25	-17	7	64	-72	9	32	-5	3	28	29
1	24	-27	5	63	57	4	28	16	H,L= 0 3			9	36	-30	H,L= 3 5			4	22	14
3	32	20	H,L= 4 1			7	50	49	2	105	-118	H,L= 2 4			3	33	44	5	38	47
5	60	-58	1	119	-112	8	58	-60	4	42	-50	0	134	128	5	22	-6	6	23	7
7	197	-174	2	123	122	9	32	-33	10	24	21	1	23	-28	6	38	44	H,L= 10 6		
9	29	-22	3	158	152	10	28	-26	H,L= 1 3			2	123	129	7	24	-26	0	82	-85
H,L= 6 0			5	125	-124	H,L= 3 2			1	44	-45	3	27	16	9	25	-25	1	43	-39
0	154	158	8	41	-39	0	93	96	3	102	-110	4	67	83	H,L= 4 5			H,L= 11 6		
2	183	179	10	43	-35	1	79	74	4	56	-60	5	29	-30	3	58	51	0	24	29
4	51	49	H,L= 5 1			2	142	-156	6	27	-19	7	31	14	5	33	-45	1	36	25
6	52	-52	1	85	84	3	109	125	8	68	-70	10	38	32	6	46	45	2	34	9
8	33	31	2	36	31	4	43	-41	10	35	39	H,L= 3 4			8	42	-46	H,L= 12 6		
10	37	40	3	77	75	5	43	46	H,L= 2 3			1	33	42	H,L= 5 5			0	24	-21
H,L= 7 0			4	50	-45	6	38	38	1	126	-127	3	50	-43	2	39	41	H,L= 14 6		
1	40	-38	5	27	-29	7	115	122	2	47	-45	4	45	51	3	56	60	0	40	-36
3	39	-35	6	34	39	9	25	25	3	72	-78	5	113	-124	4	47	-50	2	22	-25
5	126	-119	9	24	-27	H,L= 4 2			5	40	41	7	25	-26	5	41	46	H,L= 1 7		
7	78	-78	H,L= 6 1			0	178	-179	7	38	-35	9	37	-49	H,L= 6 5			3	39	-34
9	30	-24	2	134	133	1	41	-38	8	48	55	H,L= 4 4			2	41	37	H,L= 2 7		
H,L= 8 0			4	26	16	2	112	-126	10	37	34	0	138	125	3	27	29	1	27	11
0	213	207	5	59	49	3	69	-79	H,L= 3 3			2	51	50	4	49	56	2	32	-32
2	109	104	10	26	-34	4	55	-57	2	81	-88	3	53	60	5	23	-15	4	25	-12
4	46	42	H,L= 7 1			7	25	17	4	41	48	4	29	-31	H,L= 7 5			5	23	3
8	23	32	1	66	66	10	28	-38	5	59	-63	7	38	-26	1	22	-24	H,L= 3 7		
10	24	29	3	74	72	H,L= 5 2			6	69	70	8	27	24	2	30	27	3	28	-10
H,L= 9 0			5	25	26	0	25	25	9	41	43	H,L= 5 4			3	29	29	H,L= 4 7		
1	45	-47	8	35	-22	2	56	51	H,L= 4 3			0	23	-29	5	34	34	2	27	-29
3	44	-46	9	47	-30	3	44	43	1	122	-123	1	26	-14	6	35	38	4	25	-17
5	92	-88	H,L= 8 1			4	34	-33	2	46	-46	2	66	65	7	25	-5	5	29	-26
7	87	-81	1	33	-34	5	152	152	3	117	122	3	70	-75	H,L= 8 5			6	41	43
9	26	-14	2	85	84	6	35	30	4	101	-109	5	48	-57	1	24	-6	H,L= 5 7		
H,L= 10 0			4	44	42	7	44	57	5	23	12	7	50	-63	4	47	40	2	24	14
0	120	-108	10	32	-40	9	52	46	9	24	14	9	32	-28	H,L= 9 5			3	32	-22
2	127	128	H,L= 9 1			H,L= 6 2			10	26	33	H,L= 6 4			1	57	54	H,L= 6 7		
4	39	35	1	121	108	0	150	-148	H,L= 5 3			0	152	139	2	25	-4	1	31	-24
10	45	49	2	88	84	2	143	-149	1	33	-32	2	78	76	4	27	-9	2	22	0
H,L= 11 0			3	71	72	3	27	23	3	50	-54	3	31	29	5	27	30	3	28	11
1	38	33	5	35	26	4	52	-52	5	45	-52	4	34	42	7	30	-36	6	31	-35
3	58	-53	8	28	-11	5	23	23	9	33	29	H,L= 7 4			8	31	-37	H,L= 7 7		
5	70	-64	10	39	32	7	28	-22	H,L= 6 3			0	50	-50	H,L= 10 5			1	27	-9
7	90	-80	H,L= 10 1			10	34	-37	1	48	-52	3	50	-48	1	47	-46	2	30	-5
9	27	-15	1	77	-68	H,L= 7 2			8	40	37	5	49	-51	4	26	23	5	24	-27
H,L= 12 0			2	80	78	0	47	-40	10	28	29	7	58	-64	H,L= 11 5			H,L= 9 7		
0	137	134	4	48	45	1	23	21	H,L= 7 3			H,L= 8 4			3	35	35	1	31	34
2	143	136	H,L= 11 1			5	95	99	1	76	-84	0	90	85	5	27	23	5	26	-7
H,L= 13 0			2	75	-68	7	91	90	3	70	-73	1	28	37	6	25	16	H,L= 11 7		
3	80	-77	3	60	58	9	40	28	4	33	-37	2	60	56	H,L= 12 5			1	33	-37
5	39	36	H,L= 12 1			H,L= 8 2			7	32	23	3	48	-45	2	48	53	2	24	-25
7	99	-105	1	50	-44	0	29	-35	H,L= 8 3			H,L= 9 4			3	36	39	H,L= 0 8		
9	24	-17	2	28	22	1	37	29	2	91	-92	0	55	47	H,L= 13 5			0	76	67
H,L= 14 0			3	62	57	2	97	-99	4	36	-39	3	47	-41	1	26	23	2	24	24
0	73	73	4	24	15	3	23	-26	8	24	11	4	27	-18	2	31	17	H,L= 1 8		
2	28	29	6	26	-27	4	45	-51	9	33	22	5	50	-46	3	36	35	0	31	9
4	65	-59	8	30	-40	9	29	14	10	23	14	7	57	-61	H,L= 14 5			3	24	-34
6	22	28	H,L= 13 1			10	41	-47	H,L= 9 3			H,L= 10 4			1	31	28	H,L= 2 8		
8	31	32	3	25	31	H,L= 9 2			1	35	30	0	60	51	2	30	34	0	41	23
H,L= 15 0			4	43	42	1	39	33	2	48	49	1	35	31	5	22	18	H,L= 3 8		
1	30	32	5	41	38	3	36	33	3	72	-72	2	93	104	H,L= 15 5			0	24	11
3	112	-117	6	29	19	5	86	90	4	41	-45	8	25	-8	1	26	23	H,L= 4 8		
5	74	-70	9	31	-25	7	47	55	9	26	28	H,L= 11 4			4	22	19	0	45	51
7	34	22	H,L= 14 1			H,L= 10 2			H,L= 10 3			0	71	62	H,L= 17 5			2	34	32
H,L= 16 0			1	44	41	0	200	-212	8	39	47	1	36	35	1	36	37	H,L= 5 8		
0	66	64	3	86	-83	1	49	-51	H,L= 11 3			2	22	-17	H,L= 0 6			4	37	-39
2	49	54	4	73	75	3	34	27	5	35	-35	3	69	-68	0	31	32	H,L= 6 8		
H,L= 17 0			5	86	86	5	25	-16	7	30	18	5	48	-50	2	94	-84	0	29	27
7	39	-39	6	23	37	8	23	-26	H,L= 12 3			H,L= 12 4			H,L= 1 6			H,L= 7 8		
H,L= 18 0			H,L= 15 1			H,L= 11 2			1	26	27	0	42	38	0	43	-34	1	23	10
0	77	78	3	48	44	0	52	-54	3	32	43	2	23	34	1	26	12	3	34	-36
4	25	33	5	61	68	2	32	-27	4	47	-53	8	26	34	3	32	29	H,L= 8 8		
6	49	-40	6	40	-45	5	58	64	5	57	-60	H,L= 13 4			5	43	46	0	48	49
H,L= 19 0			H,L= 16 1			7	49	56	8	27	16	2	23	-15	7	43	54	2	37	39
5	35	-34	1	45	49	9	34	45	H,L 13 3			7	72	-77	H,L= 2 6			H,L= 9 8		
H,L= 20 0			4	27	33	H,L= 12 2			1	28	-32	H,L= 14 4			0	83	-67	1	26	5
0	22	2	5	47	-45	0	130	-123	3	32	-43	0	39	33	1	27	-12			
2	25	25	H,L= 17 1			1	37	-43	4	44	-45	2	72	78	2	77	-71			
H,L= 21 0			6	26	-17	2	41	-36	5	28	-26	4	27	25	3	28	13			
1	25	-1	7	24	-25	3	46	39	6	34	-48	6	26	-22	8	22	-21			
H,L= 0 1			H,L= 18 1			4	37	-32	H,L= 14 3			H,L= 15 4			H,L= 3 6					

TABLE 3. FINAL POSITIONAL AND THERMAL PARAMETERS WITH THEIR ESTIMATED STANDARD DEVIATIONS IN PARENTHESES ($\times 10^4$)

The anisotropic temperature factors are expressed in the form of $\exp\{-(B_{11}h^2+B_{22}k^2+B_{33}l^2+B_{12}hk+B_{13}hl+B_{23}kl)\}$.

Atom	x/a	y/b	z/c	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Cl (1)	0 (0)	807 (6)	7500 (0)	27 (2)	61 (6)	175 (12)	0 (0)	−59 (11)	0 (0)
Cl (2)	0 (0)	4976 (7)	7500 (0)	38 (2)	56 (5)	185 (13)	0 (0)	43 (13)	0 (0)
C (1)	2312 (8)	3715 (15)	9841 (21)	20 (5)	54 (18)	113 (29)	−23 (17)	35 (23)	11 (45)
C (2)	2714 (10)	2768 (19)	10392 (25)	31 (7)	74 (21)	199 (44)	−6 (22)	30 (27)	2 (57)
C (3)	3398 (8)	2669 (15)	9891 (25)	15 (5)	51 (16)	186 (36)	4 (15)	4 (25)	8 (49)
C (4)	3649 (8)	3539 (15)	8868 (22)	11 (4)	49 (16)	154 (33)	−10 (16)	1 (22)	22 (45)
C (5)	3260 (8)	4527 (16)	8362 (23)	15 (4)	63 (18)	163 (35)	−13 (16)	32 (23)	59 (45)
C (6)	2579 (9)	4589 (16)	8798 (21)	20 (5)	59 (18)	138 (30)	6 (15)	−61 (25)	3 (53)
C (7)	1577 (9)	3810 (18)	10348 (25)	16 (5)	88 (20)	189 (41)	−7 (18)	23 (25)	−30 (51)
C (8)	1169 (8)	2808 (20)	9564 (23)	16 (5)	105 (22)	172 (40)	−3 (20)	2 (24)	1 (57)
N	445 (6)	2882 (14)	10022 (20)	16 (4)	71 (14)	148 (25)	−17 (15)	−14 (19)	−70 (41)
O	4292 (5)	3404 (11)	8351 (15)	13 (3)	84 (13)	178 (24)	7 (12)	9 (16)	8 (33)

TABLE 4. FINAL PARAMETERS FOR HYDROGEN ATOMS

Atom	Bound to X	x/a	y/b	z/c	B(Å^2)	X–H(Å)
H (1)	C (2)	0.250	0.210	1.110	4.2	1.01
H (2)	C (3)	0.370	0.192	1.023	4.9	1.04
H (3)	C (5)	0.345	0.518	0.760	3.6	1.01
H (4)	C (6)	0.231	0.535	0.847	5.3	1.02
H (5)	C (7)	0.137	0.459	1.004	3.0	0.97
H (6)	C (7)	0.155	0.368	1.170	2.1	1.13
H (7)	C (8)	0.133	0.184	0.997	2.4	1.14
H (8)	C (8)	0.124	0.285	0.821	3.3	1.13
H (9)	N	0.032	0.215	0.934	5.6	1.00
H (10)	N	0.034	0.353	0.924	6.5	0.97
H (11)	N	0.036	0.352	1.080	9.7	0.96
H (12)	O	0.448	0.410	0.806	4.7	0.88

distances of hydrogen-bonding, and then three hydrogen atoms were placed at proper positions on the N–H···Cl$^-$ line, assuming the N–H distance to be 1.01 Å. The final cycles of refinement, involving the hydrogen atoms with isotropic temperature factors, by the block-diagonal least-squares method dropped R to 0.114. It was thought that unfavorable outer shape of the crystal caused a rather high R factor. Observed and calculated structure factors from the last cycle are given in Table 2, and the final atomic coordinates and thermal parameters with their estimated standard deviations in Table 3 and 4. The atomic scattering factors used throughout the refinement were taken from *International Tables for X-ray Crystallography* (1962). All the numerical calculations were done on an NEAC 2200—700 computer in the computing center of this University using the programs of UNICS system.

Description and Discussion of the Structure

The interatomic distances and valency angles are shown in Fig. 1. In the phenol ring part, the mean C–C distance of 1.388 Å and the C(4)–O distance of 1.361 Å are not significantly different from those values found in L-tyrosine (1.390 and 1.369 Å),[6] L-tyrosine hydrochloride (1.391 and 1.374 Å)[7] and DL-tyrosine (1.393 and 1.371 Å).[8] The small distortions of the

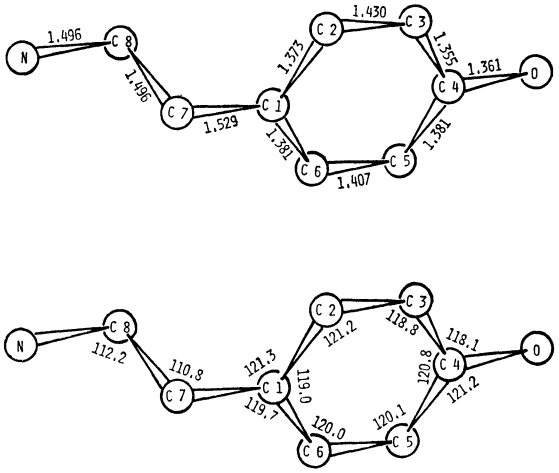

Fig. 1. Bond lengths and angles of tyramine cation. The standard deviations are 0.02 Å in bond lengths and 1.0° in bond angles between non-hydrogen atoms.

external C–C–O angles from 120° at the C(4) atom are frequently observed in phenol derivatives. The larger one always occurs at the angle C–C–O where the C–C bond is *cis* with respect to the O–H bond as suggested by Andersen *et al.*[9] The bond lengths and angles in the ethylamine side chain are very similar to the corresponding values found in other decarboxylated metabolites (amines); phenylethylamine hydrochloride,[10] dopamine hydrochloride,[11] 6-hydroxydopamine hydrochloride,[12] noradrenaline hydrochloride[13] and adrenaline hydrogen tartrate.[14]

Tyramine molecule consists of two planes; phenol ring and the fully extended ethylamine side chain. The dihedral angle between the plane of six-membered ring and the one defined by C(1)–C(7)–C(8)–N is 70.6°. The best plane through the six ring atoms was calculated by the least-squares method. The perpendicular displacements of the non-hydrogen atoms from this plane satisfying the equation: $0.2705X+0.5509Y+0.7895Z=9.8559$, are given in Table 5. The molecular conformation can be described as maximally extended form, *i.e.* the N–C(8) bond is nearly parallel to the C(7)–C(1) bond. The orientation of NH_3^+

Table 5. Deviations of atoms from the least-squares plane through the benzene ring (in Å)

Atom	Distance	Atom[a)]	Distance
C (1)	0.002	C (7)	0.013
C (2)	−0.013	C (8)	1.336
C (3)	0.003	N	1.386
C (4)	0.018	O	0.087
C (5)	−0.029	Cl (1)	4.497
C (6)	0.019	Cl (2)	2.026

a) Excluded from calculation of the plane.

group about the C(7)–C(8) bond is *trans* with respect to the C(1) atom, which is involved in the phenol ring, and the torsion angles as defined by Klyne and Prelog[15] are 179.4° (*anti-periplanar*) and 71.2° (*synclinal*) for C(1)–C(7)–C(8)–N and C(2)–C(1)–C(7)–C(8), respectively. Similar extended conformations were also reported in the crystal structures of phenylethylamine (188.9 and 72.6°),[10] dopamine (174.2 and 79.2°),[11] 6-hydroxydopamine (185.0 and 83.4°)[12] and noradrenaline (176.1 and 81.5°).[13] It is of particular interest to note that the *gauche* conformation about the C(7)–C(8) bond (the folded form) is not yet found in any crystal structure of the decarboxylated metabolite of phenylalanine and tyrosine.

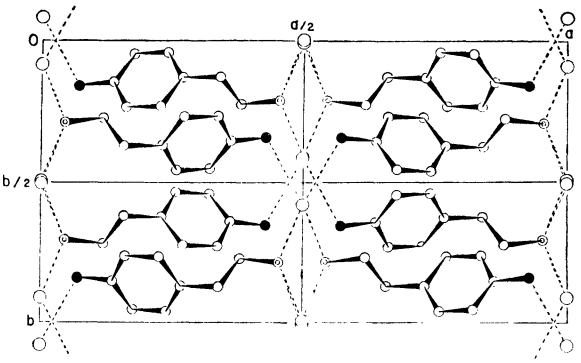

Fig. 2. The crystal structure of tyramine hydrochloride projected along the *c*-axis. The broken lines indicate the hydrogen bonds.

The packing of the molecules in this crystal is illustrated in Fig. 2, which apparently shows the network of hydrogen bonds stabilizing the structure. The crystal structure is describable as consisting of infinite chlorine layers parallel to the *bc*-plane, between which tyramine cations are arranged. The hydroxyl and ammonium hydrogen atoms are all engaged in hydrogen bonds with adjacent chlorine ions. The amino nitrogen atom has three chlorine neighbors at the distances of 3.177, 3.191, and 3.205 Å. The phenol oxygen atom acts as a donor in hydrogen bond to chlorine ion with the length of 3.028 Å. One of the interesting features of this crystal structure is the fact that two independent chlorine ions exist on the two-fold axis with distance of 4.484 Å. There is, therefore, some difference in hydrogen bonding for the two crystallographically independent chlorine ions. The Cl(2) atom is an acceptor in four N–H···Cl^- type hydrogen bonds, whereas Cl(1) acts as an acceptor of two N–H···Cl^- and two O–H···Cl^- hydrogen bonds.

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