G is a factor common to every atom in the cell. Hence the total structure factor for plane (hkl) would be

$$F(h,k,l)=G(h,k,l)\ \Sigma f_i \exp\{2\pi i(hx_i+ky_i+lz_i)\}\ ,$$

the summation being taken over all atoms in one layer, that is, half the atoms in the unit cell. The ith atom has a scattering factor of f_i.

We shall now consider the nature of the multiplier G. Summing (1) over r and q independently, we have, by the use of the binomial theorem,

$$G(h,k,l)=\sum_{n=0}^{N}(\tfrac{1}{2})^{2n}\times$$

$$\exp\left\{2\pi in\left(\frac{h}{2}+k\varepsilon_b+l\varepsilon_c\right)\{1+\exp(4\pi ik\varepsilon_b)\}^n\{1+\exp(4\pi il\varepsilon_c)\}^n\right\}$$

$$=\sum_{n=0}^{N}(\cos 2\pi k\varepsilon_b \cos 2\pi l\varepsilon_c)^n \exp(\pi inh)\ .$$

This is the sum of a geometric progression, and may be written as

$$G(h,k,l)=\frac{1-K^N\exp(\pi iNh)}{1-K\exp(\pi ih)} \qquad (2)$$

where

$$K=\cos 2\pi k\varepsilon_b \cos 2\pi l\varepsilon_c\ . \qquad (3)$$

Inspection shows that K is confined to the limits

$$-1\le K\le +1.$$

When $K=+1$

$$G(h,k,l)=\frac{\exp(-\pi iNh/2)}{\exp(-\pi ih/2)}\cdot\frac{\sin(\pi Nh/2)}{\sin(\pi h/2)}\ ,\ \text{thus}\ |G|=N$$

for even values of h.

When $K=0$

$$G(h,k,l)=1\ .$$

When $K=-1$

$$G(h,k,l)=\frac{\exp(-\pi iNh/2)}{\exp(-\pi ih/2)}\cdot\frac{\cos(\pi Nh/2)}{\cos(\pi h/2)}\ ,\ \text{thus}\ |G|=N$$

for odd values of h.

The function $\sin N\theta/\sin\theta$ is well known in diffraction theory. Since N is a very large number, when $K=1$, G is close to zero unless h is an even integer; while when $K=-1$, G is non-zero only when h is an odd integer. However, clearly when $K=0$, G is unity for all values of h, integral or non-integral. While it is more difficult to examine (2) for intermediate values of K, the above results suffice to interpret the disorder effects we have observed in the catalase crystals.

For the $h0l$ reflexions, $K=\cos 2\pi l\varepsilon_c$. When l is small, $K=+1$; thus reflexions with h odd are systematically absent. Similarly when l is larger, so that $\cos 2\pi l\varepsilon_c\rightarrow -1$, reflexions with h even are systematically absent. When l is intermediate, K is close to zero causing weak diffuse streaks parallel to the a^* axis. It then follows from Table 1 that $2\pi\,.\,5\,.\,\varepsilon_c=\pi/2$, *i.e.* $\varepsilon_c=1/20$. A similar interpretation applies to the diffuse reflexions and absences for the ($hk0$) zone; here $2\pi\,.\,7\,.\,\varepsilon_b=\pi/2$, and therefore $\varepsilon_b=1/28$. We have now determined the two unknown parameters ε_b and ε_c, and it becomes necessary to check whether their values are consistent with the other observations given in Table 1.

Let us first take the hkk reflexions. For these, $K=\cos \pi k/10\,.\,\cos \pi k/14$. We then see that K approaches $+1$, that is, h can only be even for $K<5$, $7<k<10$, $14<k<20$, *etc.*; while K approaches -1, that is h must be odd, for $5<k<7$, $10<k<14$, *etc.* Table 1 shows this to be the general appearance of the hkk reflexions, although the theoretical expected limits are not in complete agreement with the experimental results. The $h1l$ and $hk1$ reflexions should follow the same general pattern as ($h0l$) and ($hk0$) zones, although the diffuse bands might be expected to be broader in view of the fact that K cannot attain its maximum value of ± 1. Again observations are in general agreement, although the position of the diffuse streaks are not in exactly the predicted positions. Our two assumptions are thus able to predict the approximate, but not exact, position of diffuse streaks on the photographs and the nature of the unusual systematic absence.

We are grateful to Dr D. M. Blow for first pointing out the similarity of the diffraction pattern described in this paper to that observed by Dr M. F. Perutz in his study of imidazole methaemoglobin. We are also grateful to Dr M. F. Perutz for stimulating discussions as to the possible nature of the disorder. Finally we greatly appreciated not only the help Dr R. E. Marsh has given us in making the manuscript more readable, but particularly some astute comments which have put the interpretation of the disorder effect on a sounder basis.

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The crystal structure of tetraethylammineplatinum(II) dibromotetraethylammineplatinum(IV) tetrabromide.

By B. M. Craven and D. Hall*, *Crystallography Laboratory, University of Pittsburgh, Pennsylvania, U.S.A.*

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The crystal structure determination of Wolffram's red salt (Craven & Hall, 1961) confirmed earlier suggestions (Reihlen & Flohr, 1934) that it is correctly formulated $\mathrm{Pt^{II}(etn)_4\,.\,Pt^{IV}(etn)_4Cl_2\,.\,Cl_4\,.\,4H_2O}$, where etn represents an ethylamine ligand. The octahedral Pt(IV) complex ion and the square planar Pt(II) ion alternate in chains of the form $\mathrm{Cl\text{–}Pt^{IV}\text{–}Cl}$ ------ $\mathrm{Pt^{II}}$ ------ $\mathrm{Cl\text{–}Pt^{IV}\text{–}Cl}$ ------ $\mathrm{Pt^{II}}$ ------ characterized by weak charge transfer bonds from the halogen to the Pt(II) ion. The details of the molecular

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* Present address: Chemistry Department, University of Auckland, New Zealand.

structure were obscured by the extensive disorder in the crystal structure which appears to be typical of this class of compound. The interpretation of the structure rested heavily on the observation of weak diffuse layer lines recorded on oscillation photographs, and the crystal structure of the bromine analogue was undertaken because of the more intense diffraction effects to be expected if this structure is again disordered.

Orange crystals of $Pt(etn)_4 . Pt(etn)_4Br_2 . Br_4$ were obtained by slow evaporation of a solution of Wolffram's red salt in excess dilute hydrobromic acid. X-ray photographs again showed evidence of disorder, although this was of a different nature from that in Wolffram's red salt. The crystals were tetragonal, with a subcell (corresponding to the normal reflections) of dimensions $a=11{\cdot}86$, $c=12{\cdot}14$ Å, whence $d_c=4{\cdot}11$ g.cm^{-3} for 2 formula units per subcell. The odd layer lines on rotation photographs about **c** showed normal reflections superposed on a continuous diffuse background. Weissenberg photographs of these odd layers showed diffuse reflections that could be described in terms of a superlattice with a *C*-centered subcell of dimensions $2a$, $2b$, c. (The symbols H, K will hereafter be used when it is intended that the indices refer to the supercell). In addition to the normal subcell reflections (H and K even) and weak diffuse supercell reflections (H and K both odd), there was also more or less continuous diffuse streaking corresponding to reciprocal lattice lines with H odd and lines with K odd. The intensities of these diffuse lines and spots on the Weissenberg photographs, relative to those of the subcell reflections, varied considerably from crystal to crystal, and for one crystal they did not appear at all. It appears that the structure is strictly periodic only along **c**, with a somewhat variable tendency towards order in other directions.

Systematic absences in the subcell reflections were observed for $hk0$ when $h+k$ is odd, $0kl$ when l is odd, and hhl when l is odd, these being consistent with the space group $P4/ncc$. The initial interpretation of the structure was, however, made not in this space group but in $P4cc$, *i.e.* it was assumed that there is not an n-glide normal to **c**, but rather two crystallographically independent units in the subcell, such that to every atom there is a like atom related by a vector $\frac{1}{2}, \frac{1}{2}, z$. Only at the conclusion of this work was it appreciated that, within experimental error, the final structure of the subcell could be better described in terms of the space group $P4/ncc$. The coordinates reported herein are as for $P4/ncc$, but are in fact the mean of those obtained from the refinement in $P4cc$.

The subcell structure was readily deduced from the three-dimensional Patterson function and from subsequent heavy-atom phased Fourier syntheses. Chains of $Pt(etn)_4$ groups, connected by bromine atoms, occur parallel to **c**. These are as in Fig. 1, except that in the subcell there is no distinction between Pt(II) and Pt(IV), all $Pt(etn)_4$ groups appearing to have two half-weight bromines axially coordinated. Normal weight bromide ions exist independently, as shown in Fig. 2. It was assumed, as with other compounds of this type, that the chains are indeed as in Fig. 1, *i.e.* that they contain alternately 4-coordinate Pt(II) and 6-coordinate Pt(IV). The result of the disorder in the structure is then to average two chains which are nearly identical but in which the Pt(II) and Pt(IV) atoms are transposed. It seems rational to suppose that in the supercell (for which a and b are doubled), such chains occur in alternate subcells.

It was observed during refinement of the structure that both coordinated and ionic bromines showed approximately isotropic thermal motion, whereas the platinum atoms were abnormally anisotropic, requiring parameters B_{11} $(=B_{22})=0{\cdot}8$ Å^2, $B_{33}=6{\cdot}2$ Å^2. It seemed unlikely that these represent genuine thermal motion, and more probable that the platinum atoms were also affected by the disorder, and were randomly occupying two sites with slightly different z coordinate. The platinum atoms were replaced by two half-weight atoms, with isotropic B values of $0{\cdot}8$ Å^2, and structure factors were calculated for various trial separations. Optimum agreement was obtained when their z coordinates differed by $0{\cdot}46$ Å. The coordinated ethylamines must be similarly affected by the disorder, and were also described

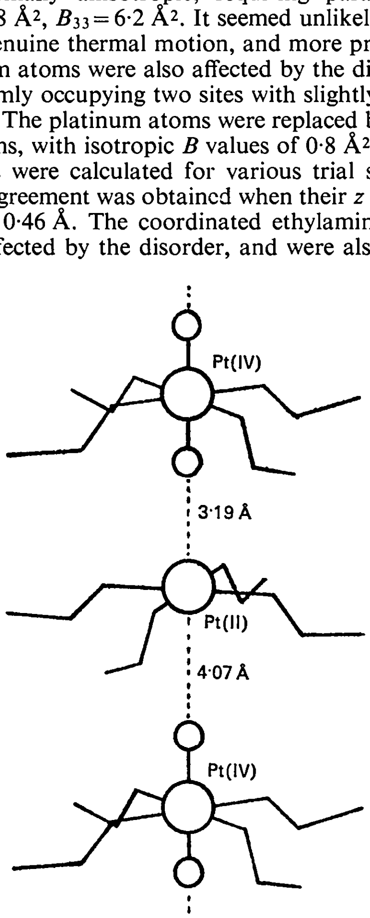

Fig. 1. A chain of alternating Pt(II) and Pt(IV) complex ions.

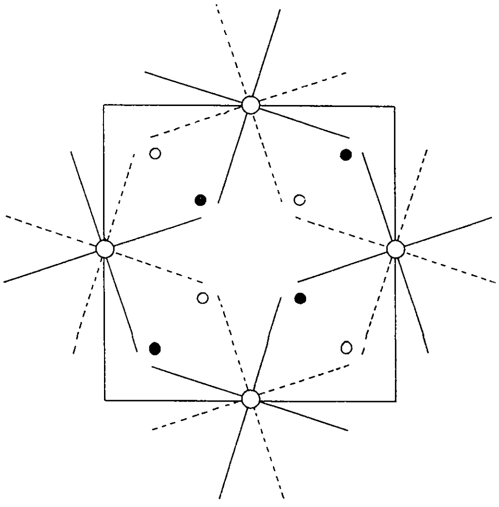

Fig. 2. Projection of the subcell on (001). The platinum atoms are shown as large circles, and bromide ions at $z=\frac{1}{4}, \frac{3}{4}$ are respectively shown as open and full small circles. The ethylamine groups attached to platinum at $z'(=0{\cdot}164\pm0{\cdot}019)$ and $\frac{1}{2}-z'$ project as full lines, those at $\frac{1}{2}+z'$ and $\bar{z}'$ as dashed lines.

in terms of half-atoms with the same separation in z. This model was refined by difference syntheses to an R index of 0·12. The final coordinates and temperature factors are listed in Table 1 (with origin at $\bar{4}$). An estimate of the accuracy is given by the application of Cruickshank's (1949) procedure to some of the parameters not affected by the disorder, *viz.* $\sigma(x)$ [$=\sigma(y)=\sigma(z)$] for the full weight bromide ion, 0·006 Å, and mean $\sigma(x)$ [$=\sigma(y)=\sigma(z)$] for the light atoms, 0·06 Å. The observed and calculated structure factors are listed in Table 2.

The bond lengths and angles involving the ethylamine ligand are: Pt–N, 2·06 Å; N–C(1), 1·40 Å; C(1)–C(2), 1·50 Å; Pt–N–C(1), 119·7°; N–C(1)–C(2), 111·7°. These appear to be normal.

Table 1. *Atom coordinates* (*origin at* $\bar{4}$) *and temperature factors*

All atoms other than Br (ionic) are half weight

Atom	x	y	z	B
Pt	0	$\frac{1}{2}$	0·144	0·8 Å^2
	0	$\frac{1}{2}$	0·182	0·8
Br	0	$\frac{1}{2}$	0·347	2·1
	0	$\frac{1}{2}$	−0·055	2·5
Br (ionic)	0·170	0·170	$\frac{1}{4}$	3·2
N	0·055	0·665	0·144	2·5
	0·055	0·665	0·182	
C(1)	0·075	0·720	0·044	3·0
	0·075	0·720	0·082	
C(2)	0·110	0·840	0·060	3·5
	0·110	0·840	0·098	

Table 2. *Observed and calculated structure factors*

Those reflections marked with an asterisk were not observed, and the value listed for F_{obs} is the maximum that would have escaped observation.

h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
2	0	0	254	257
4	0	0	213	216
6	0	0	430	448
8	0	0	148	145
10	0	0	156	162
12	0	0	245	230
14	0	0	110	110
1	1	0	270	384
3	1	0	359	474
5	1	0	299	299
7	1	0	239	221
9	1	0	264	257
11	1	0	169	154
13	1	0	186	150
15	1	0	176	134
2	2	0	203	370
4	2	0	345	390
6	2	0	247	249
8	2	0	304	285
10	2	0	221	209
12	2	0	140	137
14	2	0	186	146
3	3	0	77	74
5	3	0	336	399
7	3	0	321	331
9	3	0	123	138
11	3	0	250	230
13	3	0	193	156
15	3	0	75	81
4	4	0	315	343
6	4	0	212	202
8	4	0	253	248
10	4	0	207	203
12	4	0	147	139
14	4	0	176	141
5	5	0	218	209
7	5	0	214	207
9	5	0	236	221
11	5	0	140	144
13	5	0	164	135
6	6	0	324	323
8	6	0	149	151
10	6	0	155	153
12	6	0	203	177
14	6	0	84	91
7	7	0	184	199
9	7	0	195	195
11	7	0	140	134
13	7	0	123	114
8	8	0	201	210
10	8	0	195	165
12	8	0	112	108
9	9	0	126	124
11	9	0	193	163
10	10	0	149	139
2	1	1	93	135
3	1	1	77	78
4	1	1	191	205
5	1	1	36	34
6	1	1	24*	9
7	1	1	26*	14
8	1	1	96	77
9	1	1	31*	10
10	1	1	85	64
11	1	1	35*	0
12	1	1	35*	17
13	1	1	33*	3
14	1	1	51	28
3	2	1	6*	13
4	2	1	32	22
5	2	1	65	71
6	2	1	24*	8
7	2	1	112	104
8	2	1	29*	20
9	2	1	32	17
10	2	1	35*	15
11	2	1	66	43
13	2	1	49	30
14	2	1	29*	2
4	3	1	8*	2
5	3	1	23*	3
6	3	1	25*	7
7	3	1	28*	10
8	3	1	30*	6
9	3	1	34*	5
10	3	1	37*	0
11	3	1	38*	11
12	3	1	37*	3
13	3	1	34*	0
5	4	1	112	102
6	4	1	34	31
7	4	1	146	119
8	4	1	34*	3
9	4	1	34*	15
10	4	1	37*	5
11	4	1	79	54
12	4	1	36*	11
13	4	1	60	35
6	5	1	10*	4
7	5	1	30*	1
8	5	1	67	46
9	5	1	36*	3
10	5	1	76	48
11	5	1	38*	5
12	5	1	36*	13
13	5	1	30*	1
14	5	1	25	17
7	6	1	12*	3
8	6	1	19	14
9	6	1	37*	4
10	6	1	38*	1
11	6	1	37*	3
12	6	1	33*	1
13	6	1	27*	3
8	7	1	91	60
9	7	1	12	3
10	7	1	84	55
11	7	1	36*	0
12	7	1	30*	10
9	8	1	14*	6
10	8	1	37*	7
11	8	1	46	26
12	8	1	26*	3
10	9	1	12*	6
11	9	1	28*	3
12	9	1	20*	1
11	10	1	30	25
0	0	2	211	292
1	0	2	229	237
2	0	2	18	15
3	0	2	111	118
4	0	2	20	10
5	0	2	118	107
6	0	2	218	243
7	0	2	77	78
8	0	2	36	12
9	0	2	88	94
10	0	2	24	23
11	0	2	92	83
12	0	2	112	105
13	0	2	77	78
14	0	2	19	11
15	0	2	51	65
1	1	2	74	66
2	1	2	98	101
3	1	2	161	171
4	1	2	123	124
5	1	2	41	23
6	1	2	131	136
7	1	2	70	64
8	1	2	93	86
9	1	2	93	91
10	1	2	75	78
11	1	2	33	36
12	1	2	91	88
13	1	2	39	40
14	1	2	74	74
15	1	2	48	51
2	2	2	147	165
3	2	2	94	95
4	2	2	104	101
5	2	2	146	150
6	2	2	16	4
7	2	2	126	123
8	2	2	102	99
9	2	2	99	99
10	2	2	82	71
11	2	2	85	87
12	2	2	34	28
13	2	2	83	78
14	2	2	67	56
15	2	2	42	61
3	3	2	116	105
4	3	2	115	102
5	3	2	180	172
6	3	2	124	122
7	3	2	132	113
8	3	2	114	121
9	3	2	44	28
10	3	2	105	104
11	3	2	118	100
12	3	2	85	81
13	3	2	68	60
14	3	2	63	64
4	4	2	102	97
5	4	2	119	120
6	4	2	37	30
7	4	2	116	113
8	4	2	104	99
9	4	2	90	84
10	4	2	75	66
11	4	2	86	89
12	4	2	32	27
13	4	2	85	80
14	4	2	51	49
5	5	2	44	32
6	5	2	102	88
7	5	2	44	36
8	5	2	83	88
9	5	2	119	110
10	5	2	94	85
11	5	2	28	22
12	5	2	85	75
13	5	2	33	34
14	5	2	55	69
6	6	2	166	159
7	6	2	102	98
8	6	2	12	2
9	6	2	92	83
10	6	2	34	28
11	6	2	81	76
12	6	2	95	84
13	6	2	56	63
7	7	2	31	33
8	7	2	90	88
9	7	2	87	80
10	7	2	76	76
11	7	2	39	31
12	7	2	63	67
13	7	2	31	39
8	8	2	98	83
9	8	2	100	90
10	8	2	66	62
11	8	2	82	75
12	8	2	16*	15
9	9	2	28	4
10	9	2	87	81
11	9	2	66	65
12	9	2	49	68
10	10	2	57	51
11	10	2	52	67
2	1	3	199	217
3	1	3	15	10
4	1	3	117	118
5	1	3	27	25
6	1	3	22*	2
7	1	3	24*	7
8	1	3	84	71
9	1	3	29*	3
10	1	3	98	73
11	1	3	33*	0
12	1	3	32*	13
13	1	3	29*	7
14	1	3	35	23
3	2	3	7	13
4	2	3	31	33
5	2	3	131	126
6	2	3	32	19
7	2	3	94	83
8	2	3	27*	7
9	2	3	29*	10
10	2	3	31*	6
11	2	3	53	35
12	2	3	32*	5
13	2	3	42	37
14	2	3	24*	7
4	3	3	8*	3
5	3	3	36	24
6	3	3	33	20
7	3	3	26	12
8	3	3	28*	15
9	3	3	29*	3
10	3	3	31*	1
11	3	3	32*	5
12	3	3	31*	4
13	3	3	28*	5
5	4	3	114	112
6	4	3	19	5
7	4	3	105	81
8	4	3	28*	19
9	4	3	30*	9
10	4	3	31*	10
11	4	3	46	31
12	4	3	30*	3
13	4	3	43	39
6	5	3	11*	7
7	5	3	21	19
8	5	3	68	48
9	5	3	33*	0
10	5	3	48	40
11	5	3	33*	12
12	5	3	31*	11
13	5	3	25*	0
14	5	3	19	18
7	6	3	12*	9
8	6	3	16	7
9	6	3	33*	1
10	6	3	34*	8
11	6	3	33*	2
12	6	3	28*	1
13	6	3	22*	3
8	7	3	63	41
9	7	3	10	1
10	7	3	52	40
11	7	3	30*	0
12	7	3	25*	12
9	8	3	13*	13
10	8	3	12	3
11	8	3	30	21
12	8	3	21*	3
10	9	3	11*	21
11	9	3	2*	0
12	9	3	13*	2
11	10	3	22	19
0	0	4	30	12
1	0	4	194	199
2	0	4	233	260
3	0	4	155	167
4	0	4	180	193
5	0	4	186	182
6	0	4	11	3
7	0	4	142	166
8	0	4	148	160
9	0	4	83	84
10	0	4	101	103
11	0	4	99	100
12	0	4	48*	26
13	0	4	81	85
14	0	4	92	85
1	1	4	163	213
2	1	4	208	210
3	1	4	80	55
4	1	4	146	150
5	1	4	193	177
6	1	4	163	156
7	1	4	136	131
8	1	4	116	125
9	1	4	42	47
10	1	4	96	105
11	1	4	105	100
12	1	4	93	94
13	1	4	80	74
14	1	4	70	71
2	2	4	95	80
3	2	4	140	155
4	2	4	101	93
5	2	4	143	142
6	2	4	199	198
7	2	4	158	144
8	2	4	70	68
9	2	4	104	108
10	2	4	70	74
11	2	4	113	109
12	2	4	98	103
13	2	4	94	87
14	2	4	45	46
3	3	4	269	278
4	3	4	159	156
5	3	4	55	43
6	3	4	157	160
7	3	4	86	79
8	3	4	109	120
9	3	4	161	174
10	3	4	112	103
11	3	4	48	43
12	3	4	104	100
13	3	4	49	56
14	3	4	66	77
4	4	4	104	103
5	4	4	141	148
6	4	4	165	159
7	4	4	137	133
8	4	4	84	74
9	4	4	129	127
10	4	4	67	76
11	4	4	94	94
12	4	4	90	89
13	4	4	80	75
14	4	4	43	49
5	5	4	159	153
6	5	4	145	138
7	5	4	114	118
8	5	4	118	118
9	5	4	45	41
10	5	4	81	96
11	5	4	79	92
12	5	4	80	80
13	5	4	60	67
5	6	4	33*	3
6	6	4	6*	1
7	6	4	85	95
8	6	4	144	133
9	6	4	101	101
10	6	4	95	92
11	6	4	86	80
12	6	4	40*	22
13	6	4	50	77
7	7	4	102	94
8	7	4	102	101
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3	1	14	12	6
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4	4	14	16	5

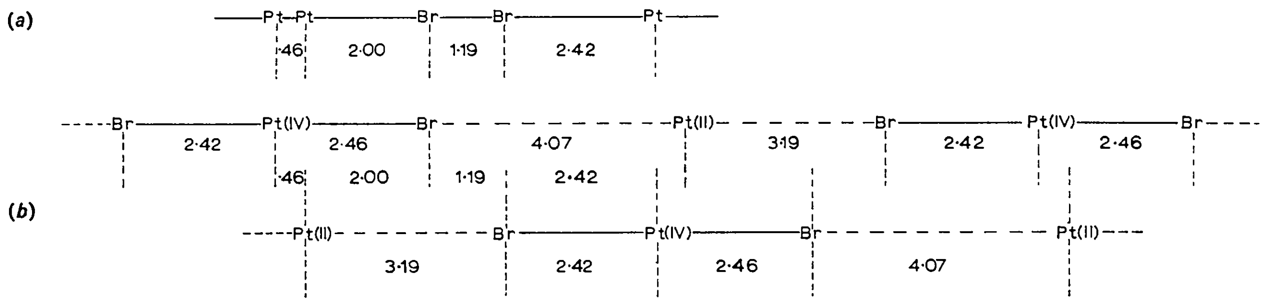

Fig. 3. (*a*) The platinum-bromide chain apparently observed. (*b*) The two chains assumed to have been averaged in (*a*).

The dimensions within the chain of half-weight platinum and bromine atoms are as in Fig. 3(*a*). If it is assumed that this is the average of two chains, in which Pt(II) and Pt(IV) alternate, then these chains are as in Fig. 3(*b*). These differ from those postulated for other compounds of this type in that the Pt(II) does not lie midway between adjacent Pt(IV) atoms, and hence the subcell appears to contain half-weight platinum as well as bromine atoms. The Pt–Br approaches in the related compound $Pt(NH_3)_2Br_2 . Pt(NH_3)_2Br_4$ (Hall & Williams, 1958) are 2·50 and 3·03 Å, the first being very close to the normal covalent bond length, and the second presumably the optimum for the charge transfer bond. In the present structure the Pt(II) atom forms one charge transfer bond only. This must lead to a greater difference in lattice energy when a stacking mistake occurs than was so for $Pt(NH_3)_2Br_2 . Pt(NH_3)_2Br_4$, but this is apparently not sufficient to prevent disorder occurring. The bond is formed on the 'open' side of the complex ion (see Fig. 1), so that repulsion between the ethylamine ligands and the bromine atom is minimized. If the two Pt---Br approaches within the chain were equal at 3·19 Å, the distance from the bromine to the four symmetry related atoms C(1) of the adjacent Pt(II) complex would be 3·50 Å instead of the observed 4·10 Å; *cf.* predicted van der Waals contact of 3·95 Å (Pauling, 1960).

The supercell will be *C*-centred, as required by the normal subcell and supercell reflections, but although square within observational limits it can only be orthorhombic in symmetry. The tetragonal diffraction symmetry observed, and the diffuse streaks, may be explained by assuming that stacking mistakes occur in which domains within the crystal are rotated by $\pi/2$ with respect to others. The *hkl* and *khl* reflections will then be averaged, and boundaries between such domains will be regions of two-dimensional order to which will correspond continuous lines in reciprocal space parallel to **a*** and **b***, and hence continuous streaks on the photographs. As far as the heavy atoms are concerned the difference between corresponding chains in adjacent subcells is a translation of $c/2$, and supercell diffraction effects will then be much more intense when l is odd.

The above phenomena are those which were observed on most photographs. However, if the mistakes were to become too frequent then not only the supercell domains but also the two-dimensional boundary regions would diminish. Both the weak reflections and the streaks would further diffuse to form continuous reciprocal lattice layers corresponding to l odd, on which would be superposed the subcell reflections. One crystal studied did correspond to this situation; *i.e.* oscillation photographs about **c** showed, for l odd, continuous layer lines with normal reflections superposed, but Weissenberg photographs showed only the subcell reflections. For most crystals both supercell reflections and streaks were apparent on Weissenberg photographs, but their intensities varied considerably. This variation within the sample studied would seem to indicate that the occurrence of growth mistakes must be sensitive to local growth conditions.

Calculations involved in this work were performed on the IBM 7070 at the University of Pittsburgh Computing Centre, using programs written by R. Shiono, P. Schapiro and R. McMullen. Atomic scattering factors used were those of Thomas & Umeda (1957) for platinum and bromine (with a real correction for dispersion in the case of platinum, and of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) for the light atoms.

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