Chadha, G. K. & Trigunayat, G. C. (1968). *Z. Kristallogr.* **126**, 86.
Jagodzinski, H. (1954). *Acta Cryst.* **7**, 300.
Jain, R. K. (1968). Ph.D. Thesis Delhi Univ.
Jain, R. K. & Trigunayat, G. C. (1968*a*). *Z. Kristallogr.* **126**, 153.
Jain, R. K. & Trigunayat, G. C. (1968*b*). *J. Crystal Growth*, **2**, 267.
Mitchell, R. S. (1955). *Phil. Mag.* **46**, 1141.
Mitchell, R. S. (1956). *Z. Kristallogr.* **108**, 296.
Ramsdell, L. S. (1944). *Amer. Min.* **29**, 431.
Srivastava, O. N. & Verma, A. R. (1962). *Z. Kristallogr.* **117**, 450.
Srivastava, O. N. & Verma, A. R. (1964). *Acta Cryst.* **17**, 260.
Srivastava, O. N. & Verma, A. R. (1965). *Acta Cryst.* **19**, 56.
Trigunayat, G. C. (1959). *Bull. N.I.S. India*, **14**, 109.

Acta Cryst. (1970). B**26**, 1791

The Conformation of Non-Aromatic Ring Compounds. LXV.* The Crystal and Molecular Structure of 3β-*p*-Bromobenzoyloxy-13α-androst-5-en-17-one

By J. C. Portheine and C. Romers

Department of Chemistry, X-ray and Electron Diffraction Section, University of Leiden, Postbox 75, Leiden, The Netherlands

(*Received* 9 *March* 1970)

The steroid 3β-*p*-bromobenzoyloxy-13α-androst-5-en-17-one crystallizes in the orthorhombic system with four molecules per unit cell. The space group is $P2_12_12_1$ and the lattice constants are $a = 16{\cdot}216 \pm 0{\cdot}006$, $b = 19{\cdot}873 \pm 0{\cdot}009$ and $c = 6{\cdot}853 \pm 0{\cdot}003$ Å. The photographic data were collected at −180°C (Cu $K\alpha$ radiation) and estimated visually. The structure was determined by application of a minimum function and by Fourier techniques. Refinement by least-squares procedures resulted in an R value of 0·117. The results of separate refinements of *a*- and *c*-axis data are discussed. The molecule has a *cis* junction between rings *C* and *D* which causes flattening of ring *C*. Ring *D* has an approximate 'envelope' conformation with the atom C(14) as flap. The *A* and *C* rings have the usual chair conformation while *B* is a 'half chair'.

Introduction

This publication is a continuation of earlier reports on the molecular geometry of steroids with various configurations at the asymmetric carbon atoms (Hesper, Geise & Romers, 1969, and papers cited therein). The title compound 3β-*p*-bromobenzoyloxy-13α-androst-5-en-17-one (hereafter APBA) has a *trans* junction between rings *B* and *C* and a *cis* junction between rings *C* and *D* (see Fig. 1). Accordingly, its configuration is 8β, 9α, 10β, 13α, 14α. The corresponding compound 3β-*p*-bromobenzoyloxy-androst-5-en-17-one with *trans* *C*/*D* coupling and belonging to the normal 8β, 9α, 10β, 13β, 14α-series will be discussed in a separate paper (Portheine, Romers & Rutten, 1970). This study was undertaken in order to investigate the conformational differences between the molecule under consideration and its 13β-isomer.

Experimental

Irradiation of the normal steroid 3β-hydroxy-androst-5-en-17-one (13β-configuration) with ultraviolet light in methanol solution induces partial conversion of the configuration at C(13) (Bots, 1958). From the isolated 13α-isomer the heavy-atom derivative APBA was prepared in benzene/pyridine solution with *p*-bromobenzoylchloride as reagent (Pot, 1964). Colourless orthorhombic needle-shaped crystals were obtained from a solution in acetone.

The unit-cell dimensions were determined from zero-layer Weissenberg photographs about [100] and the needle-axis [001]. The films were calibrated with superposed Al powder lines [a(Al) = 4·0492 Å at 20°C; λ(Cu $K\alpha_1$) = 1·54051 and λ(Cu $K\alpha_2$) = 1·54433 Å]. The observed density (flotation method) at 20°C corresponds to four molecules per unit cell (see Table 1). Absence of the odd reflexions $h00$, $0k0$ and $00l$ indicates the space group $P2_12_12_1$.

Table 1. *Crystallographic data of* APBA

3β-*p*-Bromobenzoyloxy-13α-androst-5-en-17-one	
Molecular composition	$C_{26}H_{31}BrO_3$, M = 471·4 g.mole^{-1}
Melting point	162–164°C
Space group	$P2_12_12_1$
a	16·216 (0·006) Å*
b	19·873 (0·009)
c	6·853 (0·003)
d_{obs}	1·35 (20°C)
d_{calc}	1·417 g.cm^{-3} (−180°C)
V	2208·5 Å^3

---

* Part LXIV: de Hoog & Havinga (1970).

Table 1 (*cont.*)

$F(000)$	984 electrons
Z	4 molecules.cell^{-1}
μ (Cu $K\alpha$)	29·9 cm^{-1}

* Quoted errors are twice the calculated standard deviations.

Non-integrated intensity data were collected with the equi-inclination Weissenberg multiple-film technique, using Ni-filtered Cu $K\alpha$ radiation at $-180°$C (Altona, 1964). Data were recorded from a crystal mounted about [001] (layers $l=0$–6) and from a cut crystal about [100] (layers $h=0$–9). The dimensions of the crystals were $0·15\times0·10\times1·12$ and $0·20\times0·20\times0·40$ mm respectively. In both cases the longest dimension coincided with the axis of rotation.

Altogether 2523 independent reflexions (including 337 non-observed ones) were obtained from the first crystal and 1744 (including 131 non-observed ones) from the second. The total number of possible independent reflexions in the Cu sphere is 2890.

The reduction of intensities to structure factor moduli, F_{obs}, was performed in the usual way by multiplication with the Lorentz–polarization and Phillips (1956) factors, $(\text{Lp})^{-1}$ and P respectively. No correction for absorption was applied.

Attempts were made to correlate the data from the *c*- and *a*-axis crystals by means of the scaling program of Rae (1965). The correlation can be expressed in the 'measure of agreement',

$$\sum 200|F_{\text{obs}}(a)-F_{\text{obs}}(c)|/\sum[F_{\text{obs}}(a)+F_{\text{obs}}(c)]\,,$$

which in this case amounted to 20·0%. The result is rather unsatisfactory and appears to be caused by systematic differences. This is also indicated by the overall temperature factors, which were $\exp(-1·56\sin^2\theta/\lambda^2)$ for the *a*-axis data and $\exp(-2·58\sin^2\theta/\lambda^2)$ for the *c*-axis data. Introduction of an 'extra' temperature factor, $\exp(-1·0\sin^2\theta/\lambda^2)$, into the *a*-axis data gave only a slight improvement in the correlation and was omitted afterwards. For reasons explained in the next section it was decided to keep separate data sets. During the final stages of this investigation the results of separate and simultaneous refinements of these sets were judged by statistical and chemical criteria.

Refinement

The structure was determined by the usual heavy-atom method, *i.e.* scanning of a Patterson function (based upon *c*-axis data) for the positions of the bromine atoms and application of a Buerger minimum function at these positions. Nine atoms were not located but found in a subsequent Fourier synthesis.

The two data sets were used separately for isotropic refinement of the structure by the least-squares procedure in the block-diagonal approximation. The blocks were 3×3 for positional parameters and 1×1 for the isotropic individual B values. The ten *a*-axis scaling factors were combined with an overall temperature factor in an 11×11 block. The same combination was applied to the seven *c*-axis scaling factors. The number of parameters in the respective refinements was 131 and 128.

The scattering factor used for bromine was the function evaluated by Cromer & Waber (1965); for oxygen and carbon the values were taken from *International Tables for X-ray Crystallography* (1962). For hydrogen the scattering factor values of Stewart, Davidson & Simpson (1965) were employed.

The structure amplitudes F_{obs} were weighted with a factor $w(F_{\text{obs}})=1/[a+F_{\text{obs}}+b(F_{\text{obs}})^2]$ if $F_{\text{obs}}>F_{\text{min}}$ and with $w(F_{\text{obs}})=w(F_{\text{min}})$ if $F_{\text{obs}}\le F_{\text{min}}$. Values for the parameters $a=2·00$, $b=0·20$, and $F_{\text{min}}=1·30$ in the two refinements were chosen in such a way that $\sum w(F_{\text{obs}})\times[F_{\text{obs}}-F_{\text{calc}}/S(F_{\text{obs}})]^2$ is independent of the range of F_{obs} values. F_{calc} is the modulus of the calculated structure factors on the absolute scale and $1/S(F_{\text{obs}})$ the scaling factor which reduces F_{calc} to the scale of F_{obs}.

The function $\sum w(F_{\text{obs}})\times[F_{\text{obs}}-F_{\text{calc}}/S(F_{\text{obs}})]^2$ was minimized in the refinement.

The smallest estimated intensity value (before reduction) was in this case 1·00. The non-observed reflexions were given intensities of 0·25 resulting in slightly varying values of $F'=[0·25\times(\text{Lp})^{-1}\times\text{P}]^{1/2}$ after reduction. Only if $F_{\text{calc}}/S(F')>F'$ were these reflexions included in the refinement with constant weights 0·035 (*a*-axis data) and 0·070 (*c*-axis data).

During the final cycles hydrogen atoms were introduced at calculated positions and were not refined; their B values were fixed at 1·56 and 2·58 Å^2 respectively. Convergence was reached after nine cycles for the *a*-axis data and ten cycles for the *c*-axis data. Corresponding final values for the conventional agreement index $R=\sum|F_{\text{obs}}-F_{\text{calc}}/S(F_{\text{obs}})|/\sum F_{\text{obs}}$ were $R_a=12·4\%$ and $R_c=10·8\%$.

The positional parameters resulting from these refinements were virtually the same (see next section) and suggested a simultaneous anisotropic refinement in which the reciprocal layers of each set were utilized with separate scaling factors. The dimensions of the blocks were now 3×3 for positional parameters, 6×6

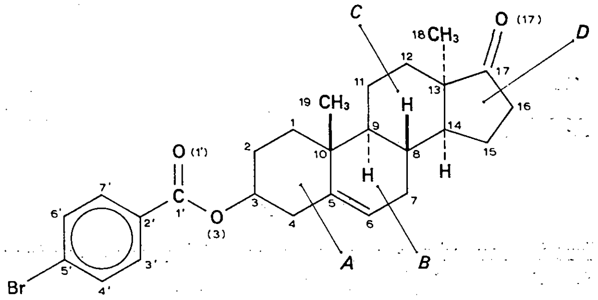


Fig. 1. Numbering of the atoms and nomenclature of 3β-*p*-bromobenzoyloxy-13α-androst-5-en-17-one (IUPAC–IUB, 1969).

for vibrational parameters and 18 × 18 for one overall isotropic temperature factor, ten *a*-axis scaling factors and seven *c*-axis factors.

The hydrogen atoms were treated as indicated before, with a B value of 2·07 Å^2. The same weighting function was used, the parameters now being $a=0·00$, $b=0·30$ and $F_{\min}=2·00$. The weight for the non-observed reflexions was 0·11. After seven cycles the shifts were smaller than one sixth of the standard deviations and the refinement was terminated. The R value was 11·7 %.

Table 2. *Fractional coordinates* × 10^4 (r_i) *of* APBA *after isotropic refinement using a- and c-axis data, their differences* Δ(10^{-3}Å), *standard deviations* $\sigma(\Delta)$ (10^{-3} Å), *final fractional coordinates* × 10^4 *after simultaneous anisotropic refinement and standard deviations* σ *in the latter* (10^{-3} Å)

	r_i	*a*-Axis	*c*-Axis	Δ	$\sigma(\Delta)$	Simultaneous	σ
C(1)	x	−1303	−1300	−7	25	−1299	9
	y	1208	1209	−2	18	1208	8
	z	3193	3193	−0	20	3191	8
C(2)	x	−529	−547	28	24	−540	9
	y	976	969	15	17	972	7
	z	2011	2040	−20	21	2019	9
C(3)	x	−803	−807	7	26	−805	9
	y	400	408	−16	17	403	7
	z	680	692	−8	21	697	8
C(4)	x	−1505	−1484	−34	25	−1489	10
	y	640	628	25	17	634	8
	z	−682	−672	−7	22	−683	9
C(5)	x	−2206	−2214	13	22	−2215	9
	y	915	910	10	16	911	7
	z	430	448	−12	22	433	8
C(6)	x	−2972	−2969	−6	25	−2966	9
	y	711	707	7	17	705	7
	z	−6	35	−28	19	2	9
C(7)	x	−3750	−3757	11	27	−3750	9
	y	957	965	−16	19	967	8
	z	930	930	1	22	938	9
C(8)	x	−3621	−3614	−10	25	−3614	9
	y	1605	1592	27	17	1600	8
	z	2200	2213	−9	20	2209	9
C(9)	x	−2807	−2792	−24	24	−2797	9
	y	1517	1530	−26	17	1521	8
	z	3341	3337	3	21	3344	8
C(10)	x	−2053	−2038	−24	25	−2038	9
	y	1450	1441	17	17	1445	7
	z	1955	1935	14	20	1953	9
C(11)	x	−2709	−2698	−17	24	−2700	9
	y	2133	2129	7	16	2128	7
	z	4767	4773	−4	21	4769	8
C(12)	x	−3393	−3396	5	24	−3396	10
	y	2141	2149	−17	18	2142	8
	z	6221	6223	−1	22	6225	9
C(13)	x	−4231	−4249	29	25	−4246	10
	y	2198	2198	−1	17	2197	7
	z	5232	5233	−5	21	5217	8
C(14)	x	−4376	−4353	−37	25	−4366	10
	y	1688	1686	5	17	1686	7
	z	3514	3552	−26	20	3533	9
C(15)	x	−5091	−5098	10	27	−5093	10
	y	1994	1999	−9	18	2000	8
	z	2371	2392	−15	23	2374	9
C(16)	x	−4930	−4926	−7	27	−4926	11
	y	2752	2755	−5	19	2753	9
	z	2460	2456	3	24	2444	10
C(17)	x	−4393	−4383	−17	25	−4390	9
	y	2875	2870	11	16	2867	7
	z	4209	4242	−23	20	4211	8
C(18)	x	−4965	−4933	−51	26	−4940	10
	y	2132	2134	−5	19	2132	9
	z	6717	6751	−23	23	6735	9
C(19)	x	−1829	−1817	−19	27	−1816	10
	y	2118	2113	11	17	2114	8
	z	883	883	0	20	897	9
C(1′)	x	464	450	23	24	447	9
	y	−212	−203	−19	17	−207	7
	z	223	233	−7	21	227	9

Table 2 (*cont.*)

	r_i	a-axis	c-axis	Δ	$\sigma(\Delta)$	Simultaneous	σ
C(2′)	x	1091	1075	27	25	1080	9
	y	−425	−440	29	18	−434	7
	z	−1173	−1145	19	21	−1165	9
C(3′)	x	1035	1041	−10	25	1035	9
	y	−289	−275	−27	18	−280	8
	z	−3190	−3130	−41	22	−3167	9
C(4′)	x	1622	1633	−18	27	1631	11
	y	−504	−508	8	19	−501	8
	z	−4424	−4388	−25	25	−4402	10
C(5′)	x	2267	2282	−25	23	2277	9
	y	−894	−884	−19	17	−890	7
	z	−3689	−3705	11	21	−3702	9
C(6′)	x	2371	2354	28	27	2361	10
	y	−1024	−1033	18	19	−1028	8
	z	−1702	−1699	−2	24	−1729	10
C(7′)	x	1737	1748	−19	28	1748	10
	y	−807	−810	7	20	−810	8
	z	−447	−425	−15	27	−464	11
O(3)	x	−114	−126	20	16	−125	6
	y	198	197	2	12	198	5
	z	−552	−547	−3	15	−557	6
O(17)	x	−4109	−4113	7	17	−4114	7
	y	3411	3398	26	13	3404	6
	z	4742	4734	5	16	4744	7
O(1′)	x	424	404	31	17	406	7
	y	−385	−386	3	13	−388	6
	z	1954	1954	−0	16	1950	7
Br	x	3097	3094	6	3	3095	1
	y	−1206	−1205	−2	2	−1206	1
	z	−5439	−5434	−4	2	−5437	1

Discussion of the refinement

The positional and thermal parameters, r_i ($i=x, y, z$ if 1, 2, 3) and B, of the separate refinements are given in Tables 2 and 3 respectively. The atom numbering is shown in Fig. 1. Table 2 indicates that for an arbitrary coordinate the absolute difference in its values resulting from the two refinements, $\Delta=[r_i(a)-r_i(c)]a_i$ ($a_i=$the corresponding lattice constant), is nowhere larger than twice its standard deviation, $\sigma(\Delta)=(\sigma_a^2+\sigma_c^2)^{1/2}$.

Table 3. *B values of* APBA *after refinement of a- and c-axis data (B_a and B_c), the difference (B_a-B_c) and the standard deviation of this difference $\sigma(B_a-B_c)$*

	B_a	B_c	B_a-B_c	$\sigma(B_a-B_c)$
C(1)	1·15 Å²	2·17 Å²	−1·02 Å²	0·30 Å²
C(2)	0·89	2·07	−1·18	0·30
C(3)	1·28	1·88	−0·60	0·31
C(4)	1·17	2·21	−1·04	0·32
C(5)	0·80	1·98	−1·18	0·27
C(6)	1·03	2·14	−1·12	0·31
C(7)	1·58	2·02	−0·44	0·34
C(8)	1·01	1·93	−0·92	0·31
C(9)	1·05	2·08	−1·03	0·31
C(10)	1·06	2·00	−0·95	0·30
C(11)	0·95	2·13	−1·18	0·30
C(12)	0·92	2·59	−1·67	0·32
C(13)	0·88	2·40	−1·52	0·30
C(14)	1·04	1·98	−0·94	0·30
C(15)	1·38	2·15	−0·78	0·33
C(16)	1·21	2·67	−1·46	0·33
C(17)	0·94	1·90	−0·96	0·30
C(18)	1·18	2·69	−1·51	0·34
C(19)	1·30	2·08	−0·78	0·31

Table 3 (*cont.*)

	B_a	B_c	B_a-B_c	$\sigma(B_a-B_c)$
C(1′)	1·20	2·11	−0·91	0·30
C(2′)	1·16	1·92	−0·76	0·31
C(3′)	1·31	2·29	−0·98	0·33
C(4′)	1·62	2·78	−1·17	0·35
C(5′)	0·83	1·98	−1·15	0·29
C(6′)	1·48	2·80	−1·32	0·36
C(7′)	2·15	2·94	−0·79	0·37
O(3)	1·17	2·03	−0·85	0·22
O(17)	1·43	2·81	−1·38	0·25
O(1′)	1·39	2·58	−1·19	0·25
Br	2·00	3·06	−1·07	0·03

It may be concluded that the positional parameter values of the two refinements are not statistically different. On the other hand, Table 3 reveals a systematic discrepancy between the B values:

$$(B_a-B_c)\simeq-3\sigma(B_a-B_c).$$

The positional parameters of the two refinements were compared by means of Hamilton's (1964) R-ratio test. This test indicates whether, at a certain significance level, the geometric model (positional parameters) of the a-axis refinement should be rejected, under the assumption that the c-axis model is correct. Using c-axis data, refinement of isotropic thermal parameters and scaling factors was carried out with fixed positional a-axis parameters. An R value $R_c'=11·3\%$ was obtained.

Consider the function $\mathcal{R}(\nu, N, \alpha)$ where ν is the number of fixed parameters ($\nu=90$), N is the number of degrees of freedom (in this case the number of observed c-axis reflexions, 2186 minus the number of parameters, 128) and α is the significance level. If the ratio R'_c/R_c is smaller than $\mathcal{R}(90, 2058, 0{\cdot}005)=1{\cdot}03$ the a-axis model cannot be rejected. The observed ratio is $11{\cdot}3/10{\cdot}8=1{\cdot}05$ which indicates rejection of the a-axis model. However, the hypothesis that the c-axis model is the correct one cannot be verified. The a-model was not therefore rejected in favour of the c-model. The R-ratio test is, strictly speaking, only valid for the generalized agreement factor (Hamilton, 1965) but may be applied to the conventional R index.

The bond lengths in the two geometric models and the corresponding standard errors are listed in Table 4. The differences in bond lengths do not exceed twice the standard deviations. Moreover, no serious deviations with respect to literature values are observed.

We assumed that the geometric models were equivalent. This equivalence is not valid for the dynamical models (vibrational parameter sets). The observed discrepancies are brought about by an accumulation of systematic errors, *i.e.* spot-shape and extinction effects and neglect of absorption in the B values. The physical meaning of these values is therefore doubtful at best.

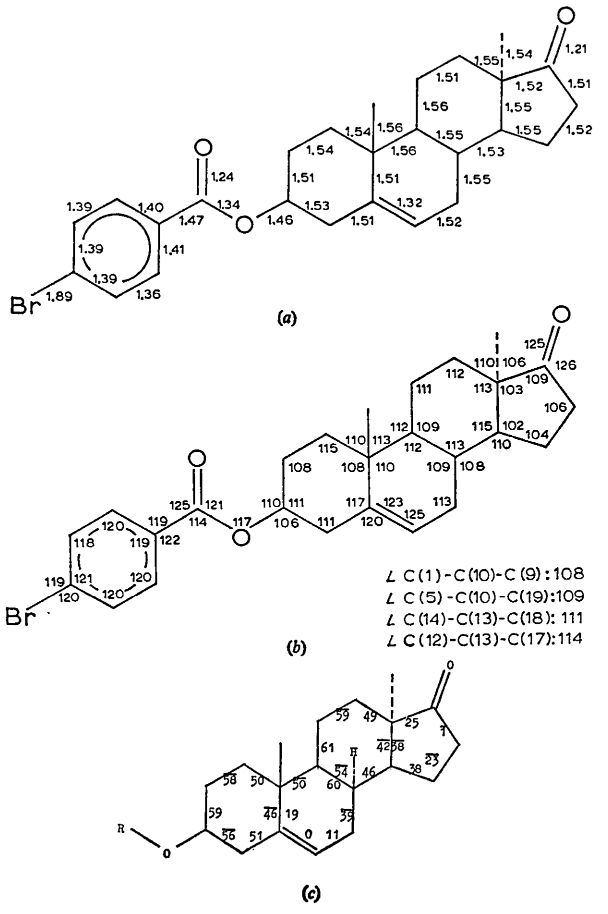


Fig. 2. (*a*) Bond lengths of APBA in Ångström units, (*b*) valency, and (*c*) torsional angles in the steroid skeleton in degrees.

Table 4. *Bond lengths* (Å) *of* APBA *and calculated standard errors* (10^{-3} Å) *after separate and simultaneous refinements*

	a-axis	c-axis	simultaneous
C(1)—C(2)	1·563 (27)	1·530 (18)	1·543 (12)
C(1)—C(10)	1·558 (28)	1·547 (18)	1·542 (12)
C(2)—C(3)	1·529 (21)	1·507 (18)	1·511 (11)
C(3)—C(4)	1·547 (28)	1·506 (18)	1·529 (13)
C(4)—C(5)	1·474 (27)	1·519 (18)	1·508 (12)
C(5)—C(6)	1·341 (29)	1·319 (15)	1·318 (12)
C(5)—C(10)	1·511 (20)	1·495 (19)	1·514 (11)
C(6)—C(7)	1·498 (30)	1·507 (17)	1·518 (12)
C(7)—C(8)	1·569 (21)	1·542 (18)	1·545 (11)
C(8)—C(9)	1·544 (29)	1·545 (17)	1·545 (12)
C(8)—C(14)	1·529 (28)	1·521 (18)	1·529 (13)
C(9)—C(10)	1·554 (28)	1·566 (18)	1·564 (13)
C(9)—C(11)	1·574 (20)	1·552 (18)	1·560 (11)
C(10)-C(19)	1·561 (21)	1·559 (17)	1·556 (11)
C(11)-C(12)	1·492 (26)	1·507 (20)	1·506 (13)
C(12)-C(13)	1·522 (29)	1·543 (19)	1·546 (14)
C(13)-C(14)	1·571 (19)	1·547 (20)	1·549 (12)
C(13)-C(17)	1·540 (19)	1·513 (17)	1·519 (10)
C(13)-C(18)	1·572 (28)	1·527 (21)	1·538 (13)
C(14)-C(15)	1·526 (29)	1·572 (18)	1·553 (13)
C(15)-C(16)	1·530 (22)	1·529 (17)	1·522 (12)
C(16)-C(17)	1·501 (25)	1·525 (21)	1·508 (13)
C(1′)-C(2′)	1·458 (26)	1·462 (19)	1·471 (13)
C(2′)-C(3′)	1·411 (21)	1·400 (22)	1·408 (13)
C(2′)-C(7′)	1·386 (29)	1·407 (17)	1·401 (13)
C(3′)-C(4′)	1·344 (29)	1·371 (20)	1·357 (14)
C(4′)-C(5′)	1·395 (27)	1·374 (17)	1·388 (13)
C(5′)-C(6′)	1·396 (21)	1·410 (23)	1·386 (14)
C(6′)-C(7′)	1·409 (30)	1·387 (21)	1·389 (14)
C(3)—O(3)	1·456 (24)	1·454 (15)	1·456 (10)
C(17)-O(17)	1·216 (19)	1·185 (13)	1·214 (10)
C(1′)-O(3)	1·352 (22)	1·339 (14)	1·340 (10)
C(1′)-O(1′)	1·237 (18)	1·237 (20)	1·236 (11)
C(5′)-Br	1·907 (18)	1·882 (13)	1·889 (9)

After six cycles of c-axis refinement a difference map was calculated. Outstanding anisotropy was observed for the bromine atom, the direction of greatest vibration being, in the plane of the benzene ring, perpendicular to the bond Br–C(5′). The thermal effects of the other atoms could not be distinguished. Nor could the hydrogen atoms be located.

Consideration of these facts prompted us to carry out the third refinement procedure mentioned in the previous section. The final positional parameters from this simultaneous refinement are listed in Table 2. The determinants of the U_{ij} tensors are positive definite for all atoms. However, due to the procedure applied, the U_{ij} values cannot have a physical meaning and are not tabulated here.* Table 5 is the final list of observed and calculated structure factors corresponding to an R value of 11·7 %. The very strong reflexions 011 and 111 from the c-axis data and 170 and 401 from the a-axis data were omitted in the last cycles of the refinement.

The geometric model of the simultaneous refinement was tested according to Hamilton using the a- and c-axis data separately. The resulting R values were $R''_a=12{\cdot}6$ % and $R''_c=10{\cdot}9$ %. The ratios $R''_a/R_a=1{\cdot}02$ and $R''_c/R_c=1{\cdot}01$ proved to be smaller than the critical

---

* A list of U_{ij} values is available upon request.

Table 5. *Observed and calculated structure factors* (FO *and* FC) *of* APBA *on four times absolute scale*

c-axis data are given first; for the non-observed reflexions (minus sign) FO × 0·7 is on four times absolute scale.

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
0	2	0	81	159	4	12	0	-21	26	8	15	0	-26	15	13	7	0	-26	17	19	10	0	49	95	3	17	1	122	153	7	16	1	174	191	12	0	1	342	339	17	6	1	163	139	2	13	2	154	158	6	14	2	128	117	10	21	2	17	25
0	4	0	425	449	4	13	0	32	39	8	16	0	131	146	13	8	0	185	178	20	0	0	22	27	3	18	1	34	31	7	17	1	59	79	12	1	1	139	124	17	7	1	29	35	2	14	2	72	62	6	15	2	149	135	11	0	2	114	95
0	6	0	227	186	4	14	0	68	68	8	17	0	51	53	13	9	0	75	73	20	1	0	35	36	3	19	1	-36	13	7	18	1	57	74	12	2	1	45	51	17	8	1	29	37	2	15	2	136	90	6	16	2	152	172	11	1	2	73	57
0	8	0	173	184	4	15	0	277	285	8	18	0	56	77	13	10	0	155	153	20	2	0	21	25	3	20	1	32	61	7	19	1	-31	15	12	3	1	88	96	17	9	1	27	26	2	16	2	121	136	6	17	2	-38	29	11	2	2	191	175
0	10	0	193	178	4	16	0	36	43	8	19	0	73	97	13	11	0	25	27	20	3	0	83	79	3	21	1	83	115	7	20	1	42	58	12	4	1	252	245	17	10	1	92	97	2	17	2	54	67	6	18	2	-36	21	11	3	2	129	139
0	12	0	420	426	4	17	0	98	106	8	20	0	116	126	13	12	0	-25	13	20	4	0	-14	13	3	22	1	23	33	7	21	1	27	31	12	5	1	119	111	17	11	1	33	27	2	18	2	76	68	6	19	2	94	107	11	4	2	125	115
0	14	0	23	30	4	18	0	64	69	8	21	0	39	32	13	13	0	-24	18	20	5	0	71	65	3	23	1	35	63	7	22	1	47	59	12	6	1	149	151	17	12	1	31	34	2	19	2	135	96	6	20	2	45	64	11	5	2	135	123
0	16	0	146	149	4	19	0	96	119	8	22	0	39	51	13	14	0	142	148	20	6	0	24	23	3	24	1	70	37	7	23	1	39	52	12	7	1	158	150	17	13	1	19	16	2	20	2	87	81	6	21	2	-29	32	11	6	2	165	127
0	18	0	129	136	4	20	0	-24	11	8	23	0	27	33	13	15	0	45	51	0	2	1	600	679	3	25	1	77	99	8	0	1	86	66	12	8	1	83	99	17	14	1	55	74	2	21	2	81	64	6	22	2	51	55	11	7	2	151	129
0	20	0	108	119	4	21	0	-23	27	9	1	0	247	225	13	16	0	16	18	0	3	1	935	947	4	0	1	561	517	8	1	1	209	243	12	9	1	93	105	18	0	1	-29	7	2	22	2	-33	29	6	23	2	58	73	11	8	2	-37	23
0	22	0	103	111	4	22	0	-21	6	9	2	0	134	117	13	17	0	-19	17	0	4	1	95	89	4	1	1	137	125	8	2	1	160	155	12	10	1	34	41	18	1	1	97	85	2	23	2	73	70	7	0	2	117	113	11	9	2	93	97
0	24	0	136	138	4	23	0	117	176	9	3	0	293	271	13	18	0	34	41	0	5	1	73	13	4	2	1	67	62	8	3	1	309	265	12	11	1	86	92	18	2	1	57	54	2	24	2	93	103	7	1	2	319	323	11	10	2	236	199
1	1	0	213	181	4	24	0	31	38	9	4	0	-20	12	13	19	0	20	29	0	6	1	284	218	4	3	1	98	99	8	4	1	70	69	12	12	1	143	157	18	3	1	59	43	3	0	2	195	171	7	2	2	236	216	11	11	2	133	123
1	2	0	58	71	4	25	0	29	42	9	5	0	293	273	14	0	0	-26	25	0	7	1	379	344	4	4	1	522	473	8	5	1	234	185	12	13	1	-33	16	18	4	1	124	135	3	1	2	139	146	7	3	2	137	135	11	12	2	132	127
1	3	0	217	161	5	1	0	32	23	9	6	0	42	36	14	1	0	92	85	0	8	1	110	85	4	5	1	143	139	8	6	1	100	108	12	14	1	56	70	18	5	1	39	35	3	2	2	244	249	7	4	2	187	196	11	13	2	53	63
1	4	0	-10	1	5	2	0	310	290	9	7	0	273	239	14	2	0	132	116	0	9	1	132	139	4	6	1	172	157	8	7	1	306	265	12	15	1	31	44	18	6	1	45	48	3	3	2	257	246	7	5	2	239	252	11	14	2	133	121
1	5	0	488	454	5	3	0	-14	19	9	8	0	159	175	14	3	0	280	239	0	10	1	265	230	4	7	1	67	61	8	8	1	-29	9	12	16	1	66	88	18	7	1	42	52	3	4	2	150	135	7	6	2	216	205	11	15	2	53	49
1	6	0	496	450	5	4	0	85	81	9	9	0	225	238	14	4	0	36	32	0	11	1	293	255	4	8	1	353	334	8	9	1	143	165	12	17	1	-27	23	18	8	1	36	40	3	5	2	177	152	7	7	2	172	147	11	16	2	33	59
1	7	0	313	294	5	5	0	163	164	9	10	0	-24	25	14	5	0	-26	11	0	12	1	53	51	4	9	1	61	59	8	10	1	78	73	12	18	1	61	77	18	9	1	64	65	3	6	2	379	305	7	8	2	172	146	11	17	2	66	63
1	8	0	109	95	5	6	0	387	349	9	11	0	35	37	14	6	0	26	26	0	13	1	41	43	4	10	1	215	173	8	11	1	181	191	12	19	1	9	23	18	10	1	-21	10	3	7	2	279	261	7	9	2	254	246	11	18	2	73	82
1	9	0	193	225	5	7	0	89	81	9	12	0	25	33	14	7	0	118	97	0	14	1	112	110	4	11	1	49	55	8	12	1	126	124	12	20	1	50	65	18	11	1	70	72	3	8	2	156	138	7	10	2	133	124	11	19	2	53	57
1	10	0	154	146	5	8	0	19	17	9	13	0	135	139	14	8	0	156	97	0	15	1	275	286	4	12	1	155	157	8	13	1	191	195	13	0	1	67	53	18	12	1	27	34	3	9	2	57	65	7	11	2	53	50	11	20	2	51	59
1	11	0	68	79	5	9	0	-19	19	9	14	0	95	91	14	9	0	-25	6	0	16	1	-33	19	4	13	1	105	95	8	14	1	68	81	13	1	1	184	164	19	0	1	-25	6	3	10	2	196	187	7	12	2	63	79	12	0	2	51	49
1	12	0	-20	9	5	10	0	439	443	9	15	0	36	64	14	10	0	-25	18	0	17	1	165	159	4	14	1	79	73	8	15	1	250	256	13	2	1	15	26	19	1	1	49	51	3	11	2	195	179	7	13	2	151	148	12	1	2	132	105
1	13	0	363	354	5	11	0	-21	21	9	16	0	-25	4	14	11	0	94	95	0	18	1	132	125	4	15	1	33	41	8	16	1	147	137	13	3	1	156	131	19	2	1	34	35	3	12	2	89	85	7	14	2	76	86	12	2	2	79	78
1	14	0	57	52	5	12	0	146	137	9	17	0	154	163	14	12	0	91	45	0	19	1	93	109	4	16	1	157	193	8	17	1	-33	36	13	4	1	-34	45	19	3	1	42	44	3	13	2	144	146	7	15	2	84	133	12	3	2	337	317
1	15	0	-24	7	5	13	0	23	39	9	18	0	70	77	14	13	0	-23	13	0	20	1	66	67	4	17	1	49	53	8	18	1	45	50	13	5	1	174	156	19	4	1	53	60	3	14	2	89	92	7	16	2	109	130	12	4	2	-37	35
1	16	0	-25	11	5	14	0	137	137	9	19	0	-22	11	14	14	0	102	100	0	21	1	-31	19	4	18	1	97	115	8	19	1	77	100	13	6	1	-34	23	19	5	1	-22	26	3	15	2	145	150	7	17	2	135	115	12	5	2	199	158
1	17	0	209	219	5	15	0	-25	11	9	20	0	79	91	14	15	0	132	121	0	22	1	70	75	4	19	1	-33	31	8	20	1	-28	23	13	7	1	183	143	19	6	1	83	76	3	16	2	132	131	7	18	2	50	27	12	6	2	157	92
1	18	0	98	111	5	16	0	97	96	9	21	0	150	133	14	16	0	63	70	0	23	1	36	47	4	20	1	159	175	8	21	1	-25	20	13	8	1	103	86	19	7	1	-20	12	3	17	2	54	67	7	19	2	33	44	12	7	2	75	53
1	19	0	106	108	5	17	0	74	68	10	0	0	285	266	14	17	0	45	53	0	24	1	-22	6	4	21	1	42	57	8	22	1	21	30	13	9	1	117	103	19	8	1	53	49	3	18	2	123	122	7	20	2	62	77	12	8	2	65	78
1	20	0	35	53	5	18	0	161	181	10	1	0	179	150	15	1	0	251	206	0	25	1	-16	9	4	22	1	97	139	8	23	1	81	98	13	10	1	-34	24	19	9	1	71	64	3	19	2	123	129	7	21	2	79	87	12	9	2	121	112
1	21	0	74	80	5	19	0	25	31	10	2	0	-21	13	15	2	0	227	152	1	0	1	192	230	4	23	1	-26	33	9	0	1	227	192	13	11	1	68	67	20	0	1	130	113	3	20	2	116	115	7	22	2	67	80	12	10	2	170	159
1	22	0	-22	1	5	20	0	34	35	10	3	0	195	184	15	3	0	-26	7	1	2	1	260	233	4	24	1	76	93	9	1	1	140	115	13	12	1	33	49	20	1	1	39	30	3	21	2	-32	5	8	0	2	436	434	12	11	2	132	96
1	23	0	-20	26	5	21	0	-22	9	10	4	0	213	185	15	4	0	117	135	1	3	1	173	139	5	0	1	32	51	9	2	1	243	220	13	13	1	137	143	20	2	1	42	45	3	22	2	134	98	8	1	2	165	155	12	12	2	-37	12
1	24	0	-17	20	5	22	0	71	76	10	5	0	110	139	15	5	0	52	53	1	4	1	283	243	5	1	1	511	441	9	3	1	78	85	13	14	1	31	39	20	3	1	-18	16	3	23	2	35	43	8	2	2	169	159	12	13	2	51	57
1	25	0	129	130	5	23	0	76	35	10	6	0	32	29	15	6	0	51	43	1	5	1	439	356	5	2	1	135	131	9	4	1	101	94	13	15	1	41	52	20	4	1	54	64	3	24	2	73	60	8	3	2	163	149	12	14	2	124	119
2	0	0	252	237	6	0	0	302	283	10	7	0	123	110	15	7	0	52	68	1	6	1	526	388	5	3	1	513	425	9	5	1	123	124	13	16	1	27	43	20	5	1	41	59	4	0	2	131	91	8	4	2	205	217	12	15	2	141	142
2	1	0	437	403	6	1	0	196	192	10	8	0	219	213	15	8	0	-25	9	1	7	1	77	85	5	4	1	237	153	9	6	1	316	270	13	17	1	92	104	0	1	2	56	53	4	1	2	64	52	8	5	2	157	155	12	16	2	46	55
2	2	0	49	36	6	2	0	42	27	10	9	0	92	92	15	9	0	66	68	1	8	1	97	92	5	5	1	335	277	9	7	1	59	62	13	18	1	-21	15	0	2	2	250	228	4	2	2	213	241	8	6	2	119	85	12	17	2	57	65
2	3	0	356	332	6	3	0	58	62	10	10	0	-25	1	15	10	0	196	195	1	9	1	272	235	5	6	1	113	93	9	8	1	43	39	13	19	1	35	40	0	3	2	131	85	4	3	2	215	229	8	7	2	122	93	12	18	2	51	55
2	4	0	978	883	6	4	0	43	56	10	11	0	186	175	15	11	0	94	101	1	10	1	427	409	5	7	1	345	311	9	9	1	-31	36	14	0	1	414	338	0	4	2	214	208	4	4	2	96	88	8	8	2	170	177	12	19	2	61	52
2	5	0	798	635	6	5	0	176	169	10	12	0	189	176	15	12	0	31	33	1	11	1	124	115	5	8	1	171	153	9	10	1	260	257	14	1	1	105	93	0	5	2	374	344	4	5	2	219	224	8	9	2	85	73	13	0	2	97	45
2	6	0	460	394	6	6	0	132	108	10	13	0	-26	26	15	13	0	60	68	1	12	1	81	85	5	9	1	435	375	9	11	1	81	70	14	2	1	105	103	0	6	2	234	171	4	6	2	223	221	8	10	2	87	83	13	1	2	53	52
2	7	0	361	344	6	7	0	193	201	10	14	0	-26	1	15	14	0	69	79	1	13	1	136	140	5	10	1	263	226	9	12	1	151	132	14	3	1	97	68	0	7	2	385	335	4	7	2	244	265	8	11	2	63	61	13	2	2	107	93
2	8	0	302	265	6	8	0	158	135	10	15	0	84	91	15	15	0	-18	16	1	14	1	252	268	5	11	1	57	73	9	13	1	-34	45	14	4	1	124	120	0	8	2	174	188	4	8	2	143	150	8	12	2	185	218	13	3	2	120	113
2	9	0	-17	0	6	9	0	188	159	10	16	0	111	139	15	16	0	-16	23	1	15	1	-32	16	5	12	1	133	111	9	14	1	140	137	14	5	1	136	140	0	9	2	-27	28	4	9	2	233	223	8	13	2	54	49	13	4	2	-59	22
2	10	0	64	59	6	10	0	95	97	10	17	0	34	37	15	17	0	26	34	1	16	1	116	111	5	13	1	157	153	9	15	1	-34	16	14	6	1	77	78	0	10	2	131	133	4	10	2	190	174	8	14	2	38	49	13	5	2	132	141
2	11	0	39	50	6	11	0	120	128	10	18	0	-22	9	16	0	0	161	156	1	17	1	-34	35	5	14	1	45	55	9	16	1	117	125	14	7	1	131	125	0	11	2	-30	23	4	11	2	253	224	8	15	2	54	73	13	6	2	121	105
2	12	0	60	70	6	12	0	258	225	10	19	0	97	98	16	1	0	86	85	1	18	1	142	155	5	15	1	33	67	9	17	1	32	51	14	8	1	131	126	0	12	2	227	186	4	12	2	-34	37	8	16	2	101	120	13	7	2	96	92
2	13	0	52	73	6	13	0	294	259	10	20	0	88	94	16	2	0	63	69	1	19	1	48	58	5	16	1	47	103	9	18	1	139	162	14	9	1	34	45	0	13	2	156	133	4	13	2	98	92	8	17	2	89	89	13	8	2	76	71
2	14	0	23	34	6	14	0	50	62	10	21	0	-16	16	16	3	0	130	132	1	20	1	84	95	5	17	1	59	81	9	19	1	29	48	14	10	1	33	41	0	14	2	-35	16	4	14	2	101	112	8	18	2	77	94	13	9	2	93	83
2	15	0	42	50	6	15	0	268	234	10	22	0	35	43	16	4	0	143	133	1	21	1	62	79	5	18	1	34	45	9	20	1	53	70	14	11	1	112	108	0	15	2	-37	69	4	15	2	179	193	8	19	2	79	97	13	10	2	235	178
2	16	0	208	194	6	16	0	229	207	11	1	0	75	64	16	5	0	25	23	1	22	1	94	125	5	19	1	-33	25	9	21	1	52	64	14	12	1	128	110	0	16	2	198	151	4	16	2	-38	35	8	20	2	102	123	13	11	2	79	75
2	17	0	26	33	6	17	0	37	63	11	2	0	325	296	16	6	0	35	43	1	23	1	36	49	5	20	1	31	65	9	22	1	27	40	14	13	1	60	74	0	17	2	291	244	4	17	2	144	141	8	21	2	51	59	13	12	2	-35	39
2	18	0	26	40	6	18	0	25	37	11	3	0	92	89	16	7	0	36	35	1	24	1	31	37	5	21	1	131	155	10	0	1	56	65	14	14	1	-28	27	0	18	2	90	97	4	18	2	37	51	8	22	2	67	82	13	13	2	36	37
2	19	0	184	208	6	19	0	214	243	11	4	0	-23	27	16	8	0	159	145	1	25	1	-16	8	5	22	1	-26	26	10	1	1	208	198	14	15	1	53	66	0	19	2	74	71	4	19	2	155	167	9	0	2	210	228	13	14	2	136	123
2	20	0	35	34	6	20	0	77	107	11	5	0	-23	3	16	9	0	-23	5	2	0	1	55	19	5	23	1	-23	15	10	2	1	99	96	14	16	1	42	43	0	20	2	179	163	4	20	2	86	87	9	1	2	191	199	13	15	2	87	89
2	21	0	24	32	6	21	0	21	34	11	6	0	171	148	16	10	0	140	123	2	1	1	527	637	5	24	1	-18	19	10	3	1	166	160	14	17	1	42	46	0	21	2	156	37	4	21	2	-31	32	9	2	2	126	97	13	16	2	59	72
2	22	0	31	39	6	22	0	44	84	11	7	0	-24	17	16	11	0	-21	13	2	2	1	412	270	6	0	1	139	154	10	4	1	199	189	14	18	1	30	31	0	22	2	87	90	4	22	2	40	52	9	3	2	172	174	13	17	2	50	45
2	23	0	92	108	6	23	0	139	149	11	8	0	102	139	16	12	0	131	124	2	3	1	461	343	6	1	1	481	375	10	5	1	71	68	15	0	1	-34	21	0	23	2	53	52	4	23	2	84	85	9	4	2	114	102	13	18	2	74	80
2	24	0	49	58	6	24	0	-13	19	11	9	0	72	71	16	13	0	26	34	2	4	1	627	458	6	2	1	328	252	10	6	1	181	173	15	1	1	69	63	0	24	2	98	84	4	24	2	-18	16	9	5	2	154	169	14	0	2	133	83
2	25	0	18	14	7	1	0	274	241	11	10	0	218	234	16	14	0	34	34	2	5	1	120	132	6	3	1	312	241	10	7	1	169	146	15	2	1	132	130	1	0	2	232	244	5	0	2	293	270	9	6	2	83	72	14	1	2	107	99
3	1	0	141	118	7	2	0	255	209	11	11	0	111	133	16	15	0	-14	7	2	6	1	247	214	6	4	1	275	212	10	8	1	200	194	15	3	1	49	56	1	1	2	247	246	5	1	2	223	224	9	7	2	145	147	14	2	2	121	101
3	2	0	347	307	7	3	0	149	133	11	12	0	52	64	16	16	0	81	75	2	7	1	226	195	6	5	1	316	223	10	9	1	125	118	15	4	1	48	51	1	2	2	264	232	5	2	2	254	264	9	8	2	137	121	14	3	2	143	182
3	3	0	260	213	7	4	0	159	144	11	13	0	146	153	17	1	0	-24	23	2	8	1	342	313	6	6	1	48	37	10	10	1	97	89	15	5	1	68	56	1	3	2	379	367	5	3	2	136	130	9	9	2	169	165	14	4	2	150	119
3	4	0	281	171	7	5	0	265	258	11	14	0	-25	8	17	2	0	18	47	2	9	1	211	254	6	7	1	85	75	10	11	1	252	252	15	6	1	144	150	1	4	2	244	212	5	4	2	87	55	9	10	2	52	55	14	5	2	54	45
3	5	0	695	522	7	6	0	212	169	11	15	0	-25	13	17	3	0	181	169	2	10	1	151	146	6	8	1	172	173	10	12	1	-34	33	15	7	1	124	112	1	5	2	300	257	5	5	2	92	69	9	11	2	75	82	14	6	2	65	57
3	6	0	513	446	7	7	0	89	195	11	16	0	60	65	17	4	0	-23	10	2	11	1	161	149	6	9	1	255	233	10	13	1	34	32	15	8	1	46	53	1	6	2	139	115	5	6	2	306	296	9	12	2	150	177	14	7	2	131	125
3	7	0	44	43	7	8	0	49	51	11	17	0	96	96	17	5	0	143	124	2	12	1	141	153	6	10	1	123	117	10	14	1	34	29	15	9	1	56	47	1	7	2	415	422	5	7	2	-27	14	9	13	2	138	141	14	8	2	83	87
3	8	0	33	27	7	9	0	242	226	11	18	0	-21	31	17	6	0	-23	1	2	13	1	140	154	6	11	1	192	157	10	15	1	48	48	15	10	1	63	58	1	8	2	292	293	5	8	2	176	165	9	14	2	95	103	14	9	2	42	75
3	9	0	334	274	7	10	0	87	91	11	19	0	-19	6	17	7	0	31	33	2	14	1	163	196	6	12	1	191	172	10	16	1	104	120	15	11	1	86	95	1	9	2	111	129	5	9	2	136	118	9	15	2	53	77	14	10	2	85	93
3	10	0	385	326	7	11	0	133	129	11	20	0	75	73	17	8	0	30	29	2	15	1	120	134	6	13	1	99	114	10	17	1	89	79	15	12	1	79	77	1	10	2	176	157	5	10	2	280	297	9	16	2	98	111	14	11	2	70	91
3	11	0	113	100	7	12	0	-24	32	11	21	0	55	67	17	9	0	124	117	2	16	1	185	210	6	14	1	71	8	10	18	1	42	61	15	13	1	55	61	1	11	2	227	209	5	11	2	173	171	9	17	2	86	92	14	12	2	33	38
3	12	0	97	92	7	13	0	221	221	12	0	0	-24	28	17	10	0	28	38	2	17	1	-34	17	6	15	1	91	93	10	19	1	104	123	15	14	1	62	74	1	12	2	214	199	5	12	2	187	188	9	18	2	-33	45	14	13	2	63	69
3	13	0	126	154	7	14	0	133	142	12	1	0	76	61	17	11	0	-19	2	2	18	1	65	92	6	16	1	270	231	10	20	1	66	82	15	15	1	-23	16	1	13	2	148	141	5	13	2	97	113	9	19	2	-30	22	14	14	2	33	34
3	14	0	372	360	7	15	0	63	74	12	2	0	128	110	17	12	0	-17	1	2	19	1	96	126	6	17	1	-36	15	10	21	1	20	38	15	16	1	45	46	1	14	2	49	39	5	14	2	176	202	9	20	2	54	69	14	15	2	67	73
3	15	0	-24	9	7	16	0	-24	37	12	3	0	320	335	17	13	0	65	39	2	20	1	73	103	6	18	1	33	37	10	22	1	21	33	15	17	1	77	64	1	15	2	52	55	5	15	2	124	137	9	21	2	32	51	14	16	2	47	63
3	16	0	68	72	7	17	0	150	160	12	4	0	217	191	18	0	0	-22	16	2	21	1	31	43	6	19	1	138	155	11	0	1	43	45	16	0	1	-33	8	1	16	2	38	46	5	16	2	94	95	9	22	2	44	56	14	17	2	29	35
3	17	0	194	184	7	18	0	63	84	12	5	0	117	137	18	1	0	44	41	2	22	1	28	40	6	20	1	126	142	11	1	1	136	146	16	1	1	97	98	1	17	2	176	152	5	17	2	-38	41	10	0	2	179	201	15	0	2	93	93
3	18	0	168	170	7	19	0	34	57	12	6	0	-25	4	18	2	0	-22	10	2	23	1	77	97	6	21	1	65	53	11	2	1	136	126	16	2	1	67	56	1	18	2	54	46	5	18	2	99	102	10	1	2	168	193	15	1	2	145	153
3	19	0	-25	21	7	20	0	-23	6	12	7	0	357	333	18	3	0	21	22	2	24	1	30	49	6	22	1	83	103	11	3	1	128	119	16	3	1	105	83	1	19	2	64	64	5	19	2	58	92	10	2	2	136	103	15	2	2	53	53
3	20	0	62	77	7	21	0	68	91	12	8	0	123	114	18	4	0	138	127	2	25	1	22	30	6	23	1	47	56	11	4	1	31	29	16	4	1	94	75	1	20	2	50	56	5	20	2	67	62	10	3	2	-33	43	15	3	2	75	67
3	21	0	-23	28	7	22	0	18	26	12	9	0	-26	19	18	5	0	-21	5	3	0	1	145	138	6	24	1	22	25	11	5	1	178	157	16	5	1	114	112	1	21	2	94	95	5	21	2	30	40	10	4	2	273	264	15	4	2	87	91
3	22	0	82	97	7	23	0	21	31	12	10	0	-26	16	18	6	0	20	26	3	1	1	172	154	7	0	1	-22	13	11	6	1	200	174	16	6	1	32	50	1	22	2	30	50	5	22	2	54	63	10	5	2	159	148	15	5	2	99	103
3	23	0	27	40	8	0	0	364	334	12	11	0	98	97	18	7	0	-19	11	3	2	1	642	472	7	1	1	192	153	11	7	1	125	110	16	7	1	92	93	1	23	2	11	14	5	23	2	54	81	10	6	2	49	57	15	6	2	-36	39
3	24	0	66	84	8	1	0	135	119	12	12	0	-26	18	18	8	0	112	103	3	3	1	581	494	7	2	1	359	295	11	8	1	66	64	16	8	1	-31	22	1	24	2	95	81	6	0	2	81	77	10	7	2	117	103	15	7	2	95	95
3	25	0	-12	24	8	2	0	-18	8	12	13	0	-25	10	18	9	0	68	53	3	4	1	242	202	7	3	1	323	249	11	9	1	227	217	16	9	1	85	87	2	0	2	425	473	6	1	2	269	293	10	8	2	157	141	15	8	2	16	73
4	0	0	238	161	8	3	0	170	117	12	14	0	35	45	18	10	0	40	44	3	5	1	493	341	7	4	1	112	105	11	10	1	93	91	16	10	1	-59	57	2	1	2	330	363	6	2	2	516	565	10	9	2	140	131	15	9	2	139	139
4	1	0	93	108	8	4	0	335	307	12	15	0	190	194	18	11	0	39	32	3	6	1	92	98	7	5	1	231	182	11	11	1	69	78	16	11	1	132	120	2	2	2	159	133	6	3	2	237	225	10	10	2	65	75	15	10	2	58	59
4	2	0	234	168	8	5	0	-19	13	12	16	0	47	49	18	12	0	81	62	3	7	1	69	62	7	6	1	450	357	11	12	1	98	98	16	12	1	-26	28	2	3	2	196	132	6	4	2	255	234	10	11	2	76	86	15	11	2	56	53
4	3	0	563	439	8	6	0	34	31	12	17	0	38	56	19	1	0	73	72	3	8	1	130	112	7	7	1	119	135	11	13	1	154	151	16	13	1	24	39	2	4	2	156	200	6	5	2	219	186	10	12	2	76	82	15	12	2	-30	22
4	4	0	121	102	8	7	0	99	88	12	18	0	27	41	19	2	0	72	70	3	9	1	334	309	7	8	1	75	64	11	14	1	115	127	16	14	1	-21	24	2	5	2	231	254	6	6	2	191	185	10	13	2	93	103	15	13	2	93	75
4	5	0	93	86	8	8	0	202	204	12	19	0	92	35	19	3	0	46	37	3	10	1	213	194	7	9	1	153	159	11	15	1	33	55	16	15	1	79	76	2	6	2	311	326	6	7	2	185	152	10	14	2	119	122	15	14	2	66	51
4	6	0	53	55	8	9	0	55	59	13	1	0	193	170	19	4	0	-18	15	3	11	1	122	126	7	10	1	170	157	11	16	1	44	62	17	0	1	45	42	2	7	2	299	268	6	8	2	193	164	10	15	2	-36	1	15	15	2	57	57
4	7	0	162	154	8	10	0	-23	1	13	2	0	271	239	19	5	0	-18	19	3	12	1	53	54	7	11	1	149	131	11	17	1	75	89	17	1	1	45	52	2	8	2	132	106	6	9	2	60	75	10	16	2	100	114	15	16	2	19	25
4	8	0	120	94	8	11	0	-24	13	13	3	0	230	169	19	6	0	-17	3	3	13	1	167	199	7	12	1	61	63	11	18	1	47	59	17	2	1	109	109	2	9	2	173	171	6	10	2	95	100	10	17	2	47	43	16	0	2	63	67
4	9	0	388	363	8	12	0	206	204	13	4	0	293	191	19	7	0	96	91	3	14	1	129	123	7	13	1	173	157	11	19	1	24	44	17	3	1	56	57	2	10	2	193	166	6	11	2	69	85	10	18	2	44	55	16	1	2	73	71
4	10	0	248	294	8	13	0	50	55	13	5	0	192	159	19	8	0	55	55	3	15	1	114	135	7	14	1	133	206	11	20	1	43	50	17	4	1	-31	18	2	11	2	253	259	6	12	2	67	72	10	19	2	69	95	16	2	2	-34	27
4	11	0	436	397	8	14	0	25	22	13	6	0	284	253	19	9	0	85	71	3	16	1	34	49	7	15	1	34	56	11	21	1	58	76	17	5	1	-30	14	2	12	2	239	230	6	13	2	164	157	10	20	2	49	67	16	3	2	-35	25

values $\mathscr{R}(90,\ 1482,\ 0{\cdot}005)=1{\cdot}04$ and $\mathscr{R}(90,\ 2058,\ 0{\cdot}005)=1{\cdot}03$ respectively. Consequently, the 'simultaneous' model cannot be rejected in comparison with the *a*- and *c*-axis models at the significance level 0·005. The geometric calculations of the molecule are therefore based on the 'simultaneous' geometric model. Moreover, it can be seen (Table 4) that for chemical reasons the 'simultaneous' model is the best.

The molecular geometry

The bond lengths and calculated standard errors are tabulated in Table 4 [see also Fig. 2(*a*)]. Systematic errors were not taken into account and, consequently, the standard errors are too small. The values of the valency and torsional angles are shown in Figs. 2(*b*) and (*c*). The average standard deviations are 0·8 and 1·2 degrees respectively.

In view of the size of the standard deviations the observed bond lengths do not differ from the expected values. This is certainly not true for the valency angles; for example C(2)–C(1)–C(10), C(8)–C(14)–C(13) and C(3)–O(3)–C(1′). The observed values are 115, 115 and 117° while the expected values are respectively 111, 110 and 110°.

The ether valency angle C(3)–O(3)–C(1′) is quite large but in agreement with recent values found in solid monochloroacetic anhydride (121°; de Kok & Romers, 1969) and in gaseous acetic anhydride (116°; Vledder, Mijlhoff, Leyte & Romers, 1970).

The distribution of torsional-angle values indicates that rings *A* and *C* are 'chairs' and ring *B* is a 'half chair'. Fig. 3 shows the Newman projections along the bond C(13)–C(14) of the compounds APBA and digitoxigenine. The latter is a recently reported steroid which also possesses a *cis* junction of the rings *C* and

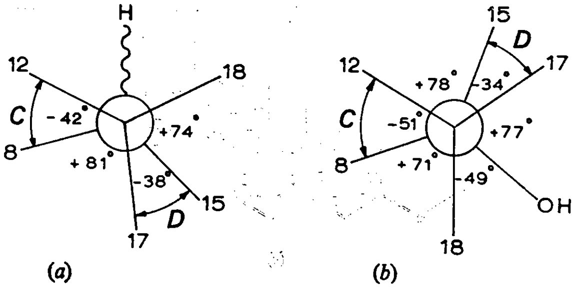


Fig. 3. Newman projections of (*a*) APBA and (*b*) digitoxigenine along the bond C(13)–C(14). Coupling of the rings *C* and *D* is indicated.

Table 5 (*cont.*)

H	K	L	FO	FC
16	4	2	89	84
16	5	2	51	72
16	6	2	60	50
16	7	2	58	69
16	8	2	104	105
16	9	2	-31	23
16	10	2	-30	19
16	11	2	-28	19
16	12	2	92	96
16	13	2	68	73
16	14	2	59	60
17	0	2	98	96
17	1	2	83	63
17	2	2	-33	12
17	3	2	94	88
17	4	2	73	63
17	5	2	102	117
17	6	2	-31	16
17	7	2	74	70
17	8	2	41	48
17	9	2	55	63
17	10	2	26	27
17	11	2	34	35
17	12	2	42	44
17	13	2	17	73
18	0	2	85	97
18	1	2	42	55
18	2	2	-29	14
18	3	2	29	36
18	4	2	64	69
18	5	2	69	70
18	6	2	-27	18
18	7	2	63	66
18	8	2	60	61
18	9	2	101	107
18	10	2	28	36
18	11	2	71	67
19	0	2	56	54
19	1	2	43	48
19	2	2	79	80
19	3	2	77	80
19	4	2	47	59
19	5	2	45	55
19	6	2	91	78
19	7	2	83	76
19	8	2	42	51
20	0	2	25	29
20	1	2	56	53
20	2	2	24	31
20	3	2	61	58
0	1	3	188	179
0	2	3	236	234
0	3	3	310	322
0	4	3	173	159
0	5	3	76	68
0	6	3	264	260
0	7	3	138	152
0	8	3	36	29
0	9	3	127	121
0	10	3	247	230
0	11	3	168	154
0	12	3	64	71
0	13	3	138	113
0	14	3	149	119
0	15	3	233	255
0	16	3	-35	30
0	17	3	-35	25
0	18	3	173	156
0	19	3	139	117
0	20	3	165	162
0	21	3	28	20
0	22	3	-25	24
0	23	3	114	90
1	0	3	222	223
1	1	3	206	201
1	2	3	232	237
1	3	3	133	125
1	4	3	160	158
1	5	3	173	185
1	6	3	185	175
1	7	3	240	245
1	8	3	98	96
1	9	3	178	177
1	10	3	239	259
1	11	3	241	240
1	12	3	45	49
1	13	3	57	62
1	14	3	194	194
1	15	3	114	126
1	16	3	93	96
1	17	3	35	43
1	18	3	34	48
1	19	3	131	121
1	20	3	30	36
1	21	3	53	62
1	22	3	35	31
1	23	3	113	85
2	0	3	126	137
2	1	3	254	252
2	2	3	145	109
2	3	3	258	255
2	4	3	169	140
2	5	3	181	159
2	6	3	228	228
2	7	3	228	216
2	8	3	186	176
2	9	3	68	82
2	10	3	185	176
2	11	3	170	170
2	12	3	45	60
2	13	3	82	96
2	14	3	139	152
2	15	3	70	87
2	16	3	149	163
2	17	3	35	40
2	18	3	100	100
2	19	3	94	95
2	20	3	75	87
2	21	3	73	81
2	22	3	75	64
2	23	3	92	70
3	0	3	246	265
3	1	3	192	175
3	2	3	141	125
3	3	3	240	220
3	4	3	307	308
3	5	3	265	229
3	6	3	220	186
3	7	3	141	136
3	8	3	176	156
3	9	3	186	190
3	10	3	144	137
3	11	3	88	97
3	12	3	161	154
3	13	3	170	164
3	14	3	65	69
3	15	3	67	79
3	16	3	154	173
3	17	3	85	101
3	18	3	64	85
3	19	3	64	66
3	20	3	79	93
3	21	3	77	77
3	22	3	33	38
3	23	3	93	61
4	0	3	339	361
4	1	3	236	216
4	2	3	43	36
4	3	3	201	172
4	4	3	260	237
4	5	3	272	228
4	6	3	34	37
4	7	3	93	86
4	8	3	163	168
4	9	3	214	227
4	10	3	74	79
4	11	3	65	37
4	12	3	181	203
4	13	3	119	135
4	14	3	60	71
4	15	3	70	70
4	16	3	67	84
4	17	3	85	101
4	18	3	-33	27
4	19	3	31	36
4	20	3	72	78
4	21	3	92	95
4	22	3	45	42
4	23	3	-17	10
5	0	3	205	201
5	1	3	138	132
5	2	3	181	179
5	3	3	127	112
5	4	3	192	193
5	5	3	180	171
5	6	3	101	90
5	7	3	190	179
5	8	3	239	249
5	9	3	114	123
5	10	3	44	33
5	11	3	92	88
5	12	3	113	123
5	13	3	116	138
5	14	3	75	82
5	15	3	-35	30
5	16	3	122	121
5	17	3	90	100
5	18	3	-33	52
5	19	3	-31	32
5	20	3	107	101
5	21	3	50	53
5	22	3	52	50
5	23	3	30	39
6	0	3	285	306
6	1	3	267	246
6	2	3	163	153
6	3	3	101	96
6	4	3	322	322
6	5	3	228	207
6	6	3	106	89
6	7	3	59	67
6	8	3	149	149
6	9	3	144	144
6	10	3	97	97
6	11	3	135	156
6	12	3	81	97
6	13	3	152	153
6	14	3	96	93
6	15	3	-35	46
6	16	3	92	91
6	17	3	75	76
6	18	3	55	63
6	19	3	96	99
6	20	3	38	52
6	21	3	58	53
6	22	3	48	52
7	0	3	129	163
7	1	3	132	114
7	2	3	200	203
7	3	3	27	44
7	4	3	169	150
7	5	3	159	163
7	6	3	227	215
7	7	3	189	178
7	8	3	107	121
7	9	3	166	183
7	10	3	158	155
7	11	3	155	156
7	12	3	69	82
7	13	3	123	120
7	14	3	115	117
7	15	3	119	119
7	16	3	68	69
7	17	3	33	35
7	18	3	53	62
7	19	3	91	87
7	20	3	-25	34
7	21	3	-22	21
7	22	3	63	57
8	0	3	-28	5
8	1	3	126	132
8	2	3	222	213
8	3	3	129	110
8	4	3	-30	31
8	5	3	117	117
8	6	3	223	216
8	7	3	65	62
8	8	3	154	154
8	9	3	58	63
8	10	3	199	192
8	11	3	49	69
8	12	3	-35	26
8	13	3	35	48
8	14	3	79	58
8	15	3	120	129
8	16	3	41	93
8	17	3	31	41
8	18	3	59	60
8	19	3	85	79
8	20	3	-23	26
8	21	3	29	33
9	0	3	43	41
9	1	3	171	176
9	2	3	116	107
9	3	3	174	175
9	4	3	44	38
9	5	3	85	79
9	6	3	155	162
9	7	3	41	78
9	8	3	58	81
9	9	3	125	119
9	10	3	206	210
9	11	3	129	120
9	12	3	-35	31
9	13	3	49	57
9	14	3	115	123
9	15	3	102	112
9	16	3	32	30
9	17	3	30	44
9	18	3	135	139
9	19	3	110	123
9	20	3	30	31
10	0	3	153	154
10	1	3	153	146
10	2	3	130	135
10	3	3	123	126
10	4	3	131	115
10	5	3	33	36
10	6	3	174	176
10	7	3	112	123
10	8	3	113	106
10	9	3	132	141
10	10	3	133	131
10	11	3	133	122
10	12	3	127	121
10	13	3	77	72
10	14	3	112	122
10	15	3	44	44
10	16	3	59	68
10	17	3	49	51
10	18	3	93	80
10	19	3	55	68
10	20	3	64	47
11	0	3	67	36
11	1	3	115	121
11	2	3	68	76
11	3	3	94	105
11	4	3	173	152
11	5	3	143	127
11	6	3	121	96
11	7	3	159	159
11	8	3	159	127
11	9	3	79	70
11	10	3	-35	31
11	11	3	60	69
11	12	3	15	16
11	13	3	112	113
11	14	3	55	82
11	15	3	43	51
11	16	3	91	86
11	17	3	63	62
11	18	3	-23	17
11	19	3	38	55
12	0	3	153	158
12	1	3	85	84
12	2	3	-35	47
12	3	3	75	86
12	4	3	103	108
12	5	3	146	145
12	6	3	61	78
12	7	3	41	58
12	8	3	118	111
12	9	3	49	51
12	10	3	69	78
12	11	3	76	71
12	12	3	146	147
12	13	3	113	107
12	14	3	-30	39
12	15	3	40	43
12	16	3	68	75
12	17	3	170	107
12	18	3	38	44
13	0	3	155	163
13	1	3	61	60
13	2	3	35	43
13	3	3	103	109
13	4	3	136	138
13	5	3	103	92
13	6	3	86	71
13	7	3	127	125
13	8	3	125	116
13	9	3	96	86
13	10	3	-33	30
13	11	3	-32	31
13	12	3	117	115
13	13	3	72	59
13	14	3	100	83
13	15	3	25	26
13	16	3	39	48
13	17	3	83	70
14	0	3	139	144
14	1	3	49	54
14	2	3	-35	25
14	3	3	70	62
14	4	3	85	86
14	5	3	68	43
14	6	3	88	91
14	7	3	82	75
14	8	3	66	64
14	9	3	117	135
14	10	3	31	31
14	11	3	93	82
14	12	3	40	45
14	13	3	105	86
14	14	3	-26	13
14	15	3	116	94
14	16	3	42	50
15	0	3	58	59
15	1	3	83	92
15	2	3	136	146
15	3	3	33	38
15	4	3	88	97
15	5	3	46	65
15	6	3	79	76
15	7	3	81	80
15	8	3	94	107
15	9	3	42	61
15	10	3	88	79
15	11	3	57	80
15	12	3	50	59
15	13	3	83	71
15	14	3	60	35
16	0	3	-31	21
16	1	3	63	67
16	2	3	93	91
16	3	3	47	50
16	4	3	-31	37
16	5	3	83	85
16	6	3	94	75
16	7	3	77	84
16	8	3	-27	27
16	9	3	66	53
16	10	3	83	76
16	11	3	72	76
16	12	3	66	60
17	0	3	28	22
17	1	3	100	81
17	2	3	90	83
17	3	3	88	78
17	4	3	-27	9
17	5	3	27	27
17	6	3	96	89
17	7	3	69	51
17	8	3	-23	11
17	9	3	-22	8
17	10	3	65	48
17	11	3	73	40
18	0	3	-24	5
18	1	3	-24	6
18	2	3	112	102
18	3	3	80	68
18	4	3	57	47
18	5	3	50	36
18	6	3	80	86
18	7	3	72	69
19	0	3	-19	5
19	1	3	75	70
19	2	3	60	63
19	3	3	91	90
19	4	3	47	45
19	5	3	37	48
0	1	4	259	247
0	2	4	59	41
0	3	4	8	12
0	4	4	109	83
0	5	4	168	142
0	6	4	-24	16
0	7	4	185	149
0	8	4	120	105
0	9	4	165	143
0	10	4	-30	3
0	11	4	109	93
0	12	4	85	51
0	13	4	173	152
0	14	4	-34	31
0	15	4	94	85
0	16	4	67	71
0	17	4	95	86
0	18	4	-31	13
0	19	4	92	85
0	20	4	77	86
0	21	4	102	96
0	22	4	52	57
1	0	4	249	257
1	1	4	46	52
1	2	4	146	108
1	3	4	176	153
1	4	4	240	228
1	5	4	110	93
1	6	4	125	110
1	7	4	220	181
1	8	4	239	214
1	9	4	80	79
1	10	4	114	104
1	11	4	71	69
1	12	4	171	153
1	13	4	98	98
1	14	4	94	92
1	15	4	69	51
1	16	4	107	105
1	17	4	92	90
1	18	4	-31	12
1	19	4	74	72
1	20	4	116	113
1	21	4	63	68
1	22	4	32	36
2	0	4	26	18
2	1	4	109	105
2	2	4	115	111
2	3	4	223	215
2	4	4	130	123
2	5	4	180	163
2	6	4	206	185
2	7	4	110	109
2	8	4	39	52
2	9	4	108	115
2	10	4	169	155
2	11	4	78	92
2	12	4	73	78
2	13	4	67	84
2	14	4	154	175
2	15	4	87	105
2	16	4	116	123
2	17	4	117	127
2	18	4	79	90
2	19	4	57	43
2	20	4	65	58
2	21	4	87	97
2	22	4	62	58
3	0	4	91	90
3	1	4	187	172
3	2	4	135	143
3	3	4	169	157
3	4	4	176	159
3	5	4	119	95
3	6	4	171	173
3	7	4	152	151
3	8	4	72	71
3	9	4	93	93
3	10	4	162	165
3	11	4	160	135
3	12	4	81	93
3	13	4	173	181
3	14	4	96	104
3	15	4	173	173
3	16	4	33	52
3	17	4	-32	43
3	18	4	-30	32
3	19	4	39	50
3	20	4	-25	26
3	21	4	-21	5
3	22	4	93	52
4	0	4	106	100
4	1	4	115	116
4	2	4	305	321
4	3	4	161	130
4	4	4	128	119
4	5	4	76	67
4	6	4	134	132
4	7	4	59	52
4	8	4	116	109
4	9	4	90	93
4	10	4	259	242
4	11	4	131	119
4	12	4	139	140
4	13	4	59	72
4	14	4	136	115
4	15	4	47	66
4	16	4	96	106
4	17	4	46	59
4	18	4	47	39
4	19	4	61	75
4	20	4	85	95
4	21	4	-20	19
4	22	4	82	97
5	0	4	95	83
5	1	4	183	152
5	2	4	100	91
5	3	4	306	277
5	4	4	93	95
5	5	4	216	201
5	6	4	175	155
5	7	4	183	150
5	8	4	189	159
5	9	4	316	331
5	10	4	225	235
5	11	4	158	141
5	12	4	47	69
5	13	4	36	32
5	14	4	-34	20
5	15	4	126	142
5	16	4	16	26
5	17	4	63	51
5	18	4	41	52
5	19	4	75	92
5	20	4	33	60
5	21	4	-13	17
6	0	4	115	105
6	1	4	197	205
6	2	4	145	139
6	3	4	165	137
6	4	4	125	123
6	5	4	58	67
6	6	4	115	129
6	7	4	135	151
6	8	4	136	137
6	9	4	96	95
6	10	4	135	111
6	11	4	47	56
6	12	4	83	85
6	13	4	93	75
6	14	4	117	126
6	15	4	-33	25
6	16	4	55	82
6	17	4	42	46
6	18	4	78	92
6	19	4	35	63
6	20	4	37	62
6	21	4	86	79
7	0	4	120	112
7	1	4	153	135
7	2	4	111	109
7	3	4	58	66
7	4	4	193	189
7	5	4	210	225
7	6	4	158	160
7	7	4	152	149
7	8	4	145	140
7	9	4	115	125
7	10	4	92	95
7	11	4	90	94
7	12	4	107	105
7	13	4	95	100
7	14	4	-33	28
7	15	4	65	53
7	16	4	87	96
7	17	4	-28	25
7	18	4	53	65
7	19	4	47	56
7	20	4	56	59
7	21	4	38	56
8	0	4	117	123
8	1	4	160	147
8	2	4	138	119
8	3	4	139	139
8	4	4	192	195
8	5	4	332	371
8	6	4	79	80
8	7	4	149	152
8	8	4	167	136
8	9	4	159	151
8	10	4	-34	29
8	11	4	-34	38
8	12	4	67	72
8	13	4	120	133
8	14	4	46	57
8	15	4	44	57
8	16	4	41	56
8	17	4	102	122
8	18	4	-24	36
8	19	4	51	49
8	20	4	29	34
9	0	4	229	258
9	1	4	63	64
9	2	4	45	40
9	3	4	108	103
9	4	4	114	117
9	5	4	46	56
9	6	4	66	73
9	7	4	104	116
9	8	4	110	118
9	9	4	34	29
9	10	4	48	55
9	11	4	33	31
9	12	4	112	122
9	13	4	32	32
9	14	4	62	92
9	15	4	29	43
9	16	4	48	62
9	17	4	25	42
9	18	4	17	28
9	19	4	26	32
10	0	4	111	108
10	1	4	128	139
10	2	4	81	90
10	3	4	81	91
10	4	4	82	93
10	5	4	67	77
10	6	4	-33	40
10	7	4	105	112
10	8	4	96	93
10	9	4	147	171
10	10	4	95	93
10	11	4	99	100
10	12	4	-32	38
10	13	4	99	170
10	14	4	84	82
10	15	4	39	58
10	16	4	36	56
10	17	4	52	58
10	18	4	28	28
11	0	4	160	150
11	1	4	58	50
11	2	4	67	70
11	3	4	96	84
11	4	4	122	133
11	5	4	76	71
11	6	4	96	83
11	7	4	117	104
11	8	4	93	83
11	9	4	125	112
11	10	4	127	123
11	11	4	108	103
11	12	4	104	93
11	13	4	59	40
11	14	4	68	64
11	15	4	111	95
11	16	4	60	62
11	17	4	28	31
11	18	4	69	70
12	0	4	48	24
12	1	4	94	81
12	2	4	140	123
12	3	4	68	62
12	4	4	48	44
12	5	4	48	43
12	6	4	130	117
12	7	4	47	44
12	8	4	90	87
12	9	4	89	74
12	10	4	106	82
12	11	4	107	85
12	12	4	-29	13
12	13	4	56	46
12	14	4	137	109
12	15	4	56	55
12	16	4	49	41
12	17	4	22	24
13	0	4	-33	2
13	1	4	130	112
13	2	4	33	33
13	3	4	113	101
13	4	4	-33	16
13	5	4	135	106
13	6	4	56	50
13	7	4	139	141
13	8	4	-31	29
13	9	4	61	49
13	10	4	72	67
13	11	4	128	101
13	12	4	-24	22
13	13	4	24	29
13	14	4	101	92
13	15	4	74	56
13	16	4	25	27
14	0	4	-32	5
14	1	4	64	65
14	2	4	85	86
14	3	4	-32	13
14	4	4	89	78
14	5	4	70	40
14	6	4	119	111
14	7	4	-30	20
14	8	4	75	72
14	9	4	39	31
14	10	4	103	91
14	11	4	25	26
14	12	4	23	23
14	13	4	91	76
14	14	4	75	72
15	0	4	131	113
15	1	4	78	77
15	2	4	-30	26
15	3	4	87	89
15	4	4	75	50
15	5	4	70	73
15	6	4	12	18
15	7	4	-29	47
15	8	4	52	56
15	9	4	79	80
15	10	4	23	29
15	11	4	37	41
15	12	4	79	60
16	0	4	55	53
16	1	4	70	64
16	2	4	38	44
16	3	4	65	55
16	4	4	45	47
16	5	4	98	73
16	6	4	35	45
16	7	4	76	64
16	8	4	61	51
16	9	4	58	45
16	10	4	18	23
16	11	4	40	41
17	0	4	90	64
17	1	4	47	51
17	2	4	66	57
17	3	4	56	53
17	4	4	123	112
17	5	4	55	50
17	6	4	59	59
17	7	4	-19	17
17	8	4	73	68
17	9	4	47	62
18	0	4	69	69
18	1	4	72	58
18	2	4	71	56
18	3	4	78	70
18	4	4	45	41
18	5	4	64	61
0	1	5	-21	26
0	2	5	306	280
0	3	5	26	19
0	4	5	-28	6
0	5	5	100	77
0	6	5	295	246
0	7	5	75	50
0	8	5	78	57
0	9	5	-36	15
0	10	5	243	227
0	11	5	38	37
0	12	5	55	58
0	13	5	-38	26
0	14	5	54	44
0	15	5	-37	26
0	16	5	72	77
0	17	5	33	49
0	18	5	140	155
0	19	5	-27	1
0	20	5	87	97
0	21	5	-15	6
1	0	5	236	194
1	1	5	244	191
1	2	5	71	53
1	3	5	193	160
1	4	5	77	63
1	5	5	123	102
1	6	5	-32	34
1	7	5	218	175
1	8	5	70	65
1	9	5	127	138
1	10	5	145	122
1	11	5	216	214
1	12	5	77	87
1	13	5	-38	9
1	14	5	94	86
1	15	5	53	73
1	16	5	-35	44
1	17	5	-16	27
1	18	5	-31	41
1	19	5	39	56
1	20	5	-23	27
1	21	5	21	33
2	0	5	95	66
2	1	5	145	127
2	2	5	170	144
2	3	5	169	148
2	4	5	-29	15
2	5	5	119	132
2	6	5	269	230
2	7	5	58	65
2	8	5	50	36
2	9	5	132	120
2	10	5	75	75
2	11	5	66	56
2	12	5	78	81
2	13	5	55	69
2	14	5	172	175
2	15	5	-37	11
2	16	5	87	82
2	17	5	58	70
2	18	5	43	43
2	19	5	-27	22
2	20	5	55	57
2	21	5	26	48
3	0	5	171	162
3	1	5	124	98
3	2	5	95	56
3	3	5	126	94
3	4	5	282	265
3	5	5	131	128
3	6	5	67	58
3	7	5	211	189
3	8	5	162	145
3	9	5	52	54
3	10	5	-38	36
3	11	5	95	99
3	12	5	95	106
3	13	5	-38	22
3	14	5	54	53
3	15	5	52	62
3	16	5	141	137
3	17	5	-33	23
3	18	5	73	85
3	19	5	59	75
3	20	5	52	80
4	0	5	114	87
4	1	5	161	172
4	2	5	61	46
4	3	5	31	39
4	4	5	102	78
4	5	5	217	216
4	6	5	121	90
4	7	5	175	158
4	8	5	52	43
4	9	5	190	157
4	10	5	54	58
4	11	5	55	61
4	12	5	-39	14
4	13	5	133	141
4	14	5	75	67
4	15	5	51	71
4	16	5	-36	20
4	17	5	64	95
4	18	5	42	44
4	19	5	43	67
4	20	5	27	29
5	0	5	307	293
5	1	5	126	106
5	2	5	125	103
5	3	5	90	62
5	4	5	159	143
5	5	5	142	123
5	6	5	136	97
5	7	5	141	111
5	8	5	131	133
5	9	5	76	74
5	10	5	54	50
5	11	5	78	80
5	12	5	245	242
5	13	5	38	38
5	14	5	37	39
5	15	5	-35	46
5	16	5	82	93
5	17	5	-31	11
5	18	5	39	54
5	19	5	23	40
5	20	5	81	112
6	0	5	92	72
6	1	5	167	171
6	2	5	120	108
6	3	5	176	162
6	4	5	137	117
6	5	5	163	152
6	6	5	138	136
6	7	5	92	67
6	8	5	-38	27
6	9	5	95	72
6	10	5	135	129
6	11	5	77	74
6	12	5	54	56
6	13	5	75	85
6	14	5	63	80
6	15	5	-36	20
6	16	5	-32	39
6	17	5	59	80
6	18	5	92	113
6	19	5	-21	21
7	0	5	161	137
7	1	5	72	70
7	2	5	-36	22
7	3	5	89	73
7	4	5	137	138
7	5	5	136	125
7	6	5	107	88
7	7	5	143	155
7	8	5	144	126
7	9	5	67	91
7	10	5	-38	15
7	11	5	109	130
7	12	5	75	74
7	13	5	73	83
7	14	5	-35	33
7	15	5	66	86
7	16	5	87	107
7	17	5	55	64
7	18	5	33	38
7	19	5	49	103
8	0	5	175	159
8	1	5	108	85
8	2	5	157	164
8	3	5	126	99
8	4	5	127	108
8	5	5	74	57
8	6	5	149	169
8	7	5	149	154
8	8	5	55	54
8	9	5	-38	42
8	10	5	109	120
8	11	5	-37	35
8	12	5	73	79
8	13	5	-35	29
8	14	5	92	106
8	15	5	-31	8
8	16	5	49	61
8	17	5	-25	25
8	18	5	29	54
9	0	5	-38	39
9	1	5	128	128
9	2	5	77	77
9	3	5	181	168
9	4	5	95	101
9	5	5	77	69
9	6	5	110	101
9	7	5	95	83
9	8	5	-38	20
9	9	5	94	96
9	10	5	65	66
9	11	5	114	131
9	12	5	-35	26
9	13	5	95	100
9	14	5	-31	20
9	15	5	101	130
9	16	5	-26	25
9	17	5	43	56
10	0	5	67	61
10	1	5	159	156
10	2	5	159	130
10	3	5	98	96
10	4	5	-39	19
10	5	5	55	66
10	6	5	109	115
10	7	5	38	49
10	8	5	-38	32
10	9	5	76	89
10	10	5	126	133
10	11	5	-35	35
10	12	5	67	73
10	13	5	44	67
10	14	5	-29	47
10	15	5	26	36
10	16	5	31	44
10	17	5	60	48
11	0	5	176	106
11	1	5	77	89
11	2	5	-38	12
11	3	5	109	101
11	4	5	121	130
11	5	5	76	59
11	6	5	-37	23
11	7	5	91	91
11	8	5	81	99
11	9	5	-35	29
11	10	5	49	72
11	11	5	-33	30
11	12	5	31	53
11	13	5	-28	20
11	14	5	26	34
11	15	5	95	97
12	0	5	-37	13
12	1	5	92	81
12	2	5	92	44
12	3	5	106	115
12	4	5	37	35
12	5	5	127	125
12	6	5	36	22
12	7	5	35	31
12	8	5	34	35
12	9	5	115	111
12	10	5	45	51
12	11	5	73	76
12	12	5	-27	14
12	13	5	61	80
12	14	5	68	75
12	15	5	62	69
13	0	5	88	83
13	1	5	-36	34
13	2	5	88	69
13	3	5	-35	12
13	4	5	222	198
13	5	5	49	46
13	6	5	33	45
13	7	5	57	54
13	8	5	127	127
13	9	5	30	45
13	10	5	40	39
13	11	5	26	10
13	12	5	23	36
14	0	5	-33	18
14	1	5	47	61
14	2	5	-33	49
14	3	5	65	57
14	4	5	32	39
14	5	5	31	58
14	6	5	43	63
14	7	5	29	41
14	8	5	-28	4
14	9	5	144	109
14	10	5	36	45
14	11	5	29	35
14	12	5	56	66
15	0	5	127	116
15	1	5	51	55
15	2	5	51	44
15	3	5	41	47
15	4	5	90	69
15	5	5	39	46
15	6	5	74	55
15	7	5	25	26
15	8	5	97	92
15	9	5	50	58
15	10	5	40	44
16	0	5	-25	19
16	1	5	25	28
16	2	5	78	85
16	3	5	48	40
17	0	5	-17	4
17	1	5	69	71
17	2	5	40	40
17	3	5	51	56
0	1	6	45	36
0	2	6	-25	4
0	3	6	95	95
0	4	6	93	66
0	5	6	160	164
0	6	6	80	58
0	7	6	-34	37
0	8	6	70	47
0	9	6	203	227
0	10	6	-36	24
0	11	6	-36	8
0	12	6	59	43
0	13	6	85	77
0	14	6	-33	8
0	15	6	176	124
0	16	6	-28	20
0	17	6	102	114
0	18	6	-21	5
0	19	6	21	41
1	0	6	169	172
1	1	6	91	53
1	2	6	37	29
1	3	6	89	73
1	4	6	249	253
1	5	6	44	33
1	6	6	148	155
1	7	6	46	51
1	8	6	132	156
1	9	6	125	116
1	10	6	133	102
1	11	6	132	95
1	12	6	-35	25
1	13	6	-16	28
1	14	6	57	55
1	15	6	55	52
1	16	6	57	61
1	17	6	25	26
1	18	6	-20	10
2	0	6	53	39
2	1	6	137	139
2	2	6	128	112
2	3	6	125	109
2	4	6	123	95
2	5	6	91	59
2	6	6	33	44
2	7	6	85	71
2	8	6	-35	17
2	9	6	114	110
2	10	6	145	152
2	11	6	88	93
2	12	6	79	55
2	13	6	98	110
2	14	6	87	105
2	15	6	-32	6
2	16	6	-28	40
2	17	6	-25	40
2	18	6	29	27
3	0	6	142	155
3	1	6	109	87
3	2	6	127	100
3	3	6	131	126
3	4	6	111	95
3	5	6	133	121
3	6	6	-36	21
3	7	6	122	129
3	8	6	88	72
3	9	6	102	107
3	10	6	72	59
3	11	6	36	55
3	12	6	35	43
3	13	6	59	65
3	14	6	32	51
3	15	6	140	176
3	16	6	39	35
3	17	6	-26	33
3	18	6	37	45
4	0	6	56	39
4	1	6	46	39
4	2	6	143	172
4	3	6	-32	16
4	4	6	134	95
4	5	6	108	81
4	6	6	149	159
4	7	6	50	42
4	8	6	102	76
4	9	6	-35	40
4	10	6	133	135
4	11	6	-35	21
4	12	6	35	29
4	13	6	47	52
4	14	6	78	101
4	15	6	51	57
4	16	6	53	55
4	17	6	32	33
4	18	6	46	72
5	0	6	14	3
5	1	6	-33	5
5	2	6	135	79
5	3	6	135	136
5	4	6	-36	5
5	5	6	90	95
5	6	6	96	73
5	7	6	108	91
5	8	6	103	82
5	9	6	107	78
5	10	6	-35	37
5	11	6	111	117
5	12	6	-36	33
5	13	6	45	65
5	14	6	-32	30
5	15	6	99	102
5	16	6	25	41
5	17	6	22	33
6	0	6	109	113
6	1	6	132	145
6	2	6	148	173
6	3	6	35	55
6	4	6	35	15
6	5	6	36	53

D (Karle & Karle, 1969). The projections demonstrate the *cis* coupling of *C* and *D*. The atom C(18) has an α-configuration in APBA and a β-configuration in digitoxigenine.

It has been shown (Altona, Geise & Romers, 1968) that a cyclopentane-like ring in any state of its pseudorotational circuit can be characterized by its values of the parameters φ_m, the measure of puckering and δ, the phase designating the actual conformation. The conformation of a steroid *D*-ring can be described as a fixed state in that circuit, with δ confined to the range $-36°$ [C(14)-'envelope' conformation] to $+36°$ [C(13)-'envelope'] for different molecules. The value of $\delta=-34°$ in APBA corresponds to a nearly ideal 'envelope' conformation with C(14) as flap.

In steroids with *D* rings *trans*-fused to *C* rings without keto groups at C(17), φ_m is found in the range 46–50°; steroids with *trans* fusion and possessing such a keto group have somewhat flatter *D* rings with $\varphi_m \simeq 44°$ [average of four observations taken from: Braun, Hornstra & Leenhouts (1969) and from Altona, Geise & Romers (1968)]. For APBA (*cis C*/*D*) φ_m is somewhat smaller (41°).

The puckering of ring *D* in digitoxigenine ($\varphi_m=36°$) is still smaller. However, the comparison with this steroid is hardly warranted since it contains a β-hydroxyl group at C(14) and a lactone group at C(17).

The torsional angles φ(17-13-14-15) and φ(12-13-14-8) are governed by the 'equality rule' introduced by Bucourt (1964) and later discussed by Geise, Altona & Romers (1967). The observations for this molecule -38 and $-42°$, are in agreement with this rule. A 'normal' *C* ring in the 'chair' conformation demands a torsional angle $\varphi(12\text{-}13\text{-}14\text{-}8) \simeq 55°$. Consequently its conformation in APBA is strongly distorted. Since the angle φ(14-8-9-11) changes only slightly under distortion (Bucourt & Hainaut, 1965) there is no transmission of the distortion towards ring *B*. The 1,4-interactions C(11)–C(17) and C(8)–C(17) correspond to distances 3·13 and 3·13 Å. These distances would assume the extremely small values of 3·00 and 3·09 Å respectively if φ(12-13-14-8) retained the value 55°.

The double bond C(5)–C(6) dictates small values for φ(9-10-5-6) and φ(1-10-5-4). This effects the same deformation of ring *A* as observed for ring *C*.

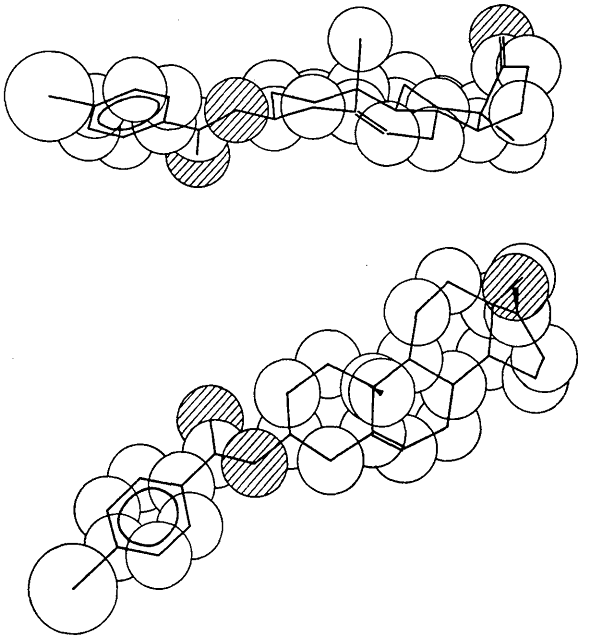
The overall-shape of the molecule (Fig. 4) is rather elongated, notwithstanding the *cis* junction of rings *C* and *D*.

The packing

A projection of the structure along [001] is shown in Fig. 5. The reference molecule I (x, y, z) is surrounded at a distance less than 4·20 Å by fourteen molecules (II–XIV) having the following coordinates:

Table 5 (*cont.*)

H	K	L	FO	FC
6	6	6	125	134
6	7	6	-36	39
6	8	6	-36	20
6	9	6	72	86
6	10	6	87	102
6	11	6	49	51
6	12	6	-33	30
6	13	6	31	46
6	14	6	41	63
6	15	6	37	41
6	16	6	40	48
7	0	6	113	128
7	1	6	-35	27
7	2	6	134	116
7	3	6	-36	31
7	4	6	153	173
7	5	6	36	33
7	6	6	36	25
7	7	6	51	56
7	8	6	88	112
7	9	6	-35	37
7	10	6	-34	32
7	11	6	58	67
7	12	6	55	71
7	13	6	42	40
7	14	6	27	33
7	15	6	69	79
7	16	6	49	69
8	0	6	-36	16
8	1	6	-36	40
8	2	6	36	31
8	3	6	89	93
8	4	6	36	21
8	5	6	89	107
8	6	6	-36	40
8	7	6	71	77
8	8	6	-35	21
8	9	6	48	71
8	10	6	-33	39
8	11	6	64	64
8	12	6	60	72
8	13	6	56	83
8	14	6	-25	12
8	15	6	52	68
9	0	6	205	193
9	1	6	72	56
9	2	6	72	52
9	3	6	51	43
9	4	6	114	91
9	5	6	71	59
9	6	6	70	45
9	7	6	-34	26
9	8	6	118	109
9	9	6	-33	3
9	10	6	45	44
9	11	6	42	30
9	12	6	137	134
9	13	6	51	30
10	0	6	-35	15
10	1	6	112	90
10	2	6	-35	51
10	3	6	100	69
10	4	6	-35	29
10	5	6	97	79
10	6	6	107	95
10	7	6	105	85
10	8	6	45	52
10	9	6	76	72
10	10	6	72	79
10	11	6	27	25
10	12	6	35	41
10	13	6	53	71
10	14	6	80	94
11	0	6	48	28
11	1	6	96	92
11	2	6	76	47
11	3	6	75	76
11	4	6	81	69
11	5	6	73	55
11	6	6	45	26
11	7	6	124	129
11	8	6	73	61
11	9	6	28	21
11	10	6	-26	35
11	11	6	117	116
11	12	6	77	59
12	0	6	-32	35
12	1	6	32	29
12	2	6	119	118
12	3	6	44	34
12	4	6	61	47
12	5	6	-30	12
12	6	6	82	92
12	7	6	39	21
12	8	6	65	46
12	9	6	-24	20
12	10	6	94	79
12	11	6	52	59
13	0	6	71	54
13	1	6	108	96
13	2	6	40	30
13	3	6	113	107
13	4	6	-27	9
13	5	6	-26	25
13	6	6	36	42
13	7	6	96	71
13	8	6	-22	40
13	9	6	54	50
13	10	6	19	24
14	0	6	35	19
14	1	6	70	68
14	2	6	129	100
14	3	6	117	105
14	4	6	32	38
14	5	6	43	48
14	6	6	109	95
15	0	6	-18	44
15	1	6	89	76
15	2	6	-17	7
15	3	6	68	42
15	4	6	51	67
0	2	0	106	159
0	4	0	405	449
0	6	0	256	186
0	8	0	223	184
0	10	0	234	179
0	12	0	561	426
0	14	0	48	30
0	16	0	231	149
0	18	0	177	136
0	20	0	154	119
0	22	0	149	111
0	24	0	192	138
0	1	1	77	57
0	2	1	508	470
0	3	1	829	847
0	4	1	96	68
0	5	1	19	13
0	6	1	272	219
0	7	1	339	344
0	8	1	103	85
0	9	1	144	139
0	10	1	267	230
0	11	1	302	255
0	12	1	69	51
0	13	1	59	40
0	14	1	134	110
0	15	1	346	284
0	16	1	-26	19
0	17	1	213	155
0	18	1	175	125
0	19	1	150	100
0	20	1	95	67
0	21	1	35	19
0	22	1	109	76
0	23	1	56	47
0	24	1	-17	6
0	25	1	18	9
0	0	2	497	562
0	1	2	47	50
0	2	2	270	225
0	3	2	74	85
0	4	2	212	205
0	5	2	354	344
0	6	2	207	171
0	7	2	352	335
0	8	2	157	189
0	9	2	-20	28
0	10	2	119	100
0	11	2	-22	20
0	12	2	183	186
0	13	2	159	133
0	14	2	-25	16
0	15	2	81	69
0	16	2	139	151
0	17	2	269	244
0	18	2	113	87
0	19	2	91	71
0	20	2	192	163
0	21	2	130	97
0	22	2	111	90
0	23	2	71	62
0	24	2	94	84
0	1	3	202	179
0	2	3	210	234
0	3	3	307	322
0	4	3	173	159
0	5	3	68	69
0	6	3	259	280
0	7	3	151	152
0	8	3	30	29
0	9	3	116	121
0	10	3	199	230
0	11	3	132	154
0	12	3	54	71
0	13	3	114	113
0	14	3	122	119
0	15	3	249	233
0	16	3	-27	30
0	17	3	-27	25
0	18	3	171	156
0	19	3	144	117
0	20	3	175	162
0	21	3	31	20
0	22	3	-19	24
0	23	3	100	90
0	0	4	194	174
0	1	4	259	247
0	2	4	52	41
0	3	4	-21	12
0	4	4	96	53
0	5	4	116	142
0	6	4	-23	16
0	7	4	133	149
0	8	4	139	135
0	9	4	140	143
0	10	4	-25	3
0	11	4	81	93
0	12	4	-27	51
0	13	4	129	152
0	14	4	-27	31
0	15	4	84	85
0	16	4	68	71
0	17	4	118	84
0	18	4	-24	13
0	19	4	108	85
0	20	4	98	84
0	21	4	111	96
0	22	4	39	57
0	1	5	-25	26
0	2	5	273	280
0	3	5	-25	19
0	4	5	-25	6
0	5	5	79	77
0	6	5	223	246
0	7	5	53	55
0	8	5	66	57
0	9	5	-27	15
0	10	5	193	227
0	11	5	27	32
0	12	5	39	58
0	13	5	27	26
0	14	5	37	44
0	15	5	-25	26
0	16	5	71	77
0	17	5	36	49
0	18	5	153	155
0	19	5	-18	1
0	20	5	97	87
0	0	6	-27	21
0	1	6	27	36
0	2	6	-27	4
0	3	6	84	95
0	4	6	59	54
0	5	6	142	154
0	6	6	67	58
0	7	6	-27	37
0	8	6	38	47
0	9	6	198	227
0	10	6	-26	24
0	11	6	-26	8
0	12	6	35	63
0	13	6	74	77
0	14	6	-23	8
0	15	6	127	124
0	16	6	-19	23
0	17	6	113	116
0	1	7	126	142
0	2	7	64	84
0	3	7	37	54
0	4	7	-26	0
0	5	7	-25	23
0	6	7	-25	36
0	7	7	35	36
0	8	7	-26	27
0	9	7	46	49
0	10	7	74	93
0	11	7	42	55
0	12	7	39	46
0	13	7	-18	6
0	14	7	88	93
0	0	8	93	126
0	1	8	65	87
0	2	8	79	94
0	3	8	95	111
0	4	8	54	75
0	5	8	38	53
0	6	8	-15	6
0	7	8	24	40
0	8	8	44	63
0	9	8	37	58
1	2	0	61	71
1	3	0	187	161
1	4	0	-15	1
1	5	0	643	654
1	6	0	578	650
1	8	0	169	95
1	9	0	220	223
1	10	0	156	146
1	11	0	71	79
1	12	0	-28	9
1	13	0	332	354
1	14	0	64	52
1	15	0	-33	7
1	16	0	-35	11
1	17	0	198	219
1	18	0	102	111
1	19	0	108	108
1	20	0	49	53
1	21	0	81	80
1	22	0	-31	1
1	23	0	-27	26
1	24	0	-23	20
1	25	0	143	130
1	0	1	189	230
1	1	1	387	489
1	2	1	171	233
1	3	1	121	139
1	4	1	221	243
1	5	1	309	356
1	6	1	351	389
1	7	1	62	65
1	8	1	83	82
1	9	1	268	235
1	10	1	373	409
1	11	1	158	116
1	12	1	111	86
1	13	1	162	140
1	14	1	261	269
1	15	1	-34	16
1	16	1	123	111
1	17	1	-38	35
1	18	1	171	155
1	19	1	73	58
1	20	1	111	95
1	21	1	87	79
1	22	1	129	125
1	23	1	47	49
1	24	1	32	37
1	0	2	234	248
1	1	2	236	246
1	2	2	228	232
1	3	2	315	367
1	4	2	212	212
1	5	2	237	282
1	6	2	99	115
1	7	2	365	422
1	8	2	278	280
1	9	2	89	109
1	10	2	139	157
1	11	2	156	209
1	12	2	164	180
1	13	2	193	141
1	14	2	101	89
1	15	2	66	55
1	16	2	50	46
1	17	2	165	162
1	18	2	36	46
1	19	2	86	64
1	20	2	47	56
1	21	2	118	85
1	22	2	49	50
1	23	2	-25	16
1	24	2	96	81
1	0	3	227	223
1	1	3	192	231
1	2	3	226	237
1	3	3	128	129
1	4	3	136	158
1	5	3	165	183
1	6	3	153	175
1	7	3	209	245
1	8	3	83	96
1	9	3	171	177
1	10	3	240	239
1	11	3	241	240
1	12	3	58	49
1	13	3	59	62
1	14	3	237	194
1	15	3	149	126
1	16	3	121	96
1	17	3	50	43
1	18	3	69	48
1	19	3	139	121
1	20	3	44	36
1	21	3	70	62
1	22	3	44	31
1	23	3	95	83
1	0	4	229	257
1	1	4	49	47
1	2	4	118	108
1	3	4	144	153
1	4	4	223	228
1	5	4	90	93
1	6	4	159	110
1	7	4	139	181
1	8	4	213	214
1	9	4	71	79
1	10	4	105	104
1	11	4	66	69
1	12	4	160	163
1	13	4	95	98
1	14	4	85	92
1	15	4	36	51
1	16	4	100	105
1	17	4	96	90
1	18	4	-32	12
1	19	4	80	72
1	20	4	149	113
1	21	4	81	68
1	22	4	38	36
1	0	5	205	194
1	1	5	213	191
1	2	5	47	51
1	3	5	179	160
1	4	5	58	43
1	5	5	137	102
1	6	5	-34	34
1	7	5	203	195
1	8	5	71	65
1	9	5	101	108
1	10	5	117	122
1	11	5	219	214
1	12	5	85	87
1	13	5	-35	9
1	14	5	85	86
1	15	5	81	73
1	16	5	45	44
1	17	5	35	27
1	18	5	27	41
1	19	5	77	56
1	20	5	40	27
1	0	6	197	172
1	1	6	72	69
1	2	6	-36	29
1	3	6	89	70
1	4	6	256	250
1	5	6	-36	33
1	6	6	154	156
1	7	6	51	51
1	8	6	166	154
1	9	6	124	114
1	10	6	99	107
1	11	6	95	95
1	12	6	-33	33
1	13	6	-31	28
1	14	6	60	56
1	15	6	79	62
1	16	6	89	61
1	17	6	31	24
1	0	7	-34	37
1	1	7	155	124
1	2	7	69	68
1	3	7	144	115
1	4	7	83	80
1	5	7	151	120
1	6	7	70	65
1	7	7	91	78
1	8	7	44	45
1	9	7	96	71
1	10	7	29	35
1	11	7	75	61
1	12	7	36	40
1	13	7	57	53
1	14	7	65	61
1	15	7	52	41
1	0	8	-27	12
1	1	8	-27	29
1	2	8	79	69
1	3	8	-26	17
1	4	8	51	60
1	5	8	25	38
1	6	8	76	61
1	7	8	22	33
1	8	8	67	58
1	9	8	72	57
1	10	8	51	47
2	3	0	297	332
2	4	0	747	883
2	5	0	645	535
2	6	0	521	394
2	7	0	377	344
2	8	0	306	268
2	9	0	-15	0
2	10	0	67	59
2	11	0	56	50
2	12	0	84	70
2	13	0	96	73
2	14	0	40	36
2	15	0	59	50
2	16	0	237	194
2	17	0	33	33
2	18	0	52	40
2	19	0	227	258
2	20	0	42	34
2	21	0	30	32
2	22	0	49	39
2	23	0	116	108
2	24	0	73	58
2	0	1	40	19
2	1	1	355	437
2	2	1	253	273
2	3	1	286	343
2	4	1	376	459
2	5	1	116	132
2	6	1	197	216
2	7	1	185	195
2	8	1	253	313
2	9	1	232	206
2	10	1	167	145
2	11	1	155	143
2	12	1	168	153
2	13	1	189	156
2	14	1	217	185
2	15	1	162	135
2	16	1	232	213
2	17	1	-23	17
2	18	1	115	92
2	19	1	135	125
2	20	1	131	103
2	21	1	56	43
2	22	1	37	43
2	23	1	101	97
2	24	1	64	63
2	25	1	38	33
2	0	2	368	473
2	1	2	373	363
2	2	2	100	100
2	3	2	185	192
2	4	2	152	203
2	5	2	201	255
2	6	2	284	325
2	7	2	243	259
2	8	2	196	105
2	9	2	159	171
2	10	2	167	186
2	11	2	235	257
2	12	2	237	233
2	13	2	175	159
2	14	2	75	52
2	15	2	137	93
2	16	2	135	125
2	17	2	49	57
2	18	2	94	55
2	19	2	111	95
2	20	2	132	91
2	21	2	82	56
2	22	2	31	29
2	23	2	73	73
2	24	2	132	103
2	0	3	115	137
2	1	3	229	232
2	2	3	95	133
2	3	3	235	255
2	4	3	133	143
2	5	3	133	133
2	6	3	213	229
2	7	3	213	215
2	8	3	180	175
2	9	3	74	92
2	10	3	148	175
2	11	3	154	173
2	12	3	62	63
2	13	3	96	95
2	14	3	139	152
2	15	3	133	37
2	16	3	195	153
2	17	3	57	69
2	18	3	111	133
2	19	3	135	95
2	20	3	99	82
2	21	3	105	81
2	22	3	73	54
2	23	3	69	73
2	0	4	-15	13
2	1	4	133	105
2	2	4	197	111
2	3	4	203	215
2	4	4	138	123
2	5	4	137	143
2	6	4	181	185
2	7	4	125	139
2	8	4	52	52
2	9	4	109	113
2	10	4	165	155
2	11	4	103	92
2	12	4	99	78
2	13	4	43	93
2	14	4	199	175
2	15	4	139	105
2	16	4	148	123
2	17	4	147	127
2	18	4	111	93
2	19	4	43	83
2	20	4	73	39
2	21	4	117	92
2	22	4	75	59
2	0	5	57	55
2	1	5	131	122
2	2	5	147	146
2	3	5	150	148
2	4	5	-22	15
2	5	5	102	102
2	6	5	220	230
2	7	5	75	65
2	8	5	43	34
2	9	5	110	120
2	10	5	95	75
2	11	5	57	54
2	12	5	78	81
2	13	5	66	68
2	14	5	167	175
2	15	5	-21	11
2	16	5	85	82
2	17	5	80	70
2	18	5	42	43
2	19	5	21	22
2	20	5	63	57
2	0	6	40	38
2	1	6	143	138
2	2	6	125	112
2	3	6	117	108
2	4	6	98	95
2	5	6	86	69
2	6	6	55	44
2	7	6	90	71
2	8	6	-23	17
2	9	6	109	110
2	10	6	147	152
2	11	6	86	93
2	12	6	59	66
2	13	6	120	110
2	14	6	119	104
2	15	6	-17	4
2	16	6	48	40
2	17	6	49	40
2	18	6	35	27
2	0	7	-22	2
2	1	7	106	104
2	2	7	55	61
2	3	7	89	86
2	4	7	58	63
2	5	7	133	153
2	6	7	120	126
2	7	7	76	76
2	8	7	50	53
2	9	7	64	77
2	10	7	37	42
2	11	7	24	26
2	12	7	23	32
2	13	7	82	83
2	14	7	82	77
2	15	7	43	28
2	0	8	32	34
2	1	8	49	55
2	2	8	75	75
2	3	8	74	73
2	4	8	83	80
2	5	8	52	58
2	6	8	43	53
2	7	8	49	53
2	8	8	39	45
2	9	8	53	54
3	1	0	89	118
3	2	0	250	307
3	3	0	207	213
3	4	0	214	171
3	5	0	498	522
3	6	0	445	446
3	7	0	45	43
3	8	0	36	27
3	9	0	200	274
3	10	0	341	326
3	11	0	176	100
3	12	0	116	92
3	13	0	151	134
3	14	0	370	360
3	15	0	-22	9
3	16	0	101	72
3	17	0	228	184
3	18	0	213	170
3	19	0	23	21
3	20	0	84	77
3	21	0	30	28
3	22	0	120	97
3	23	0	57	40
3	24	0	94	84
3	0	1	117	138
3	1	1	119	154
3	2	1	348	472
3	3	1	410	494
3	4	1	193	202
3	5	1	287	341
3	6	1	103	98
3	7	1	91	62
3	8	1	125	112
3	9	1	330	309
3	10	1	208	194
3	11	1	154	126
3	12	1	67	54
3	13	1	208	188
3	14	1	140	123
3	15	1	161	135
3	16	1	43	40
3	17	1	272	163
3	18	1	33	31
3	19	1	-23	13
3	20	1	41	43
3	21	2	-20	5
3	22	1	39	39
3	23	1	61	49
3	24	1	49	37
3	0	2	156	171
3	1	2	125	146
3	2	2	197	249
3	3	2	234	246
3	4	2	119	135
3	5	2	130	152
3	6	2	369	395
3	7	2	285	261
3	8	2	129	138
3	9	2	61	65
3	10	2	184	187
3	11	2	165	178
3	12	2	89	80
3	13	2	183	146
3	14	2	97	92
3	15	2	200	160
3	16	2	164	131
3	17	2	81	67
3	18	2	151	122
3	19	2	151	129
3	20	2	142	115
3	21	2	9	5
3	22	2	106	98
3	23	2	51	43
3	24	2	42	40
3	0	3	225	265
3	1	3	154	175
3	2	3	104	125
3	3	3	199	220
3	4	3	247	308
3	5	3	188	229
3	6	3	191	196
3	7	3	120	136
3	8	3	129	156
3	9	3	150	180
3	10	3	121	137
3	11	3	97	97
3	12	3	158	154
3	13	3	162	166
3	14	3	77	69
3	15	3	86	79
3	16	3	204	173
3	17	3	113	101
3	18	3	102	85
3	19	3	83	66
3	20	3	114	93
3	21	3	97	77
3	22	3	34	38
3	23	3	75	61
3	0	4	78	90
3	1	4	154	172
3	2	4	131	140
3	3	4	149	162
3	4	4	145	158
3	5	4	90	95
3	6	4	92	103
3	7	4	145	151
3	8	4	73	71
3	9	4	89	93
3	10	4	127	145
3	11	4	130	135
3	12	4	84	83
3	13	4	168	181
3	14	4	110	104
3	15	4	192	173
3	16	4	72	52
3	17	4	53	40
3	18	4	36	37
3	19	4	77	60
3	20	4	24	24
3	21	4	-15	5
3	22	4	64	52
3	0	5	169	167
3	1	5	99	98
3	2	5	67	56
3	3	5	88	94
3	4	5	265	269
3	5	5	102	108
3	6	5	44	58
3	7	5	168	189
3	8	5	137	143
3	9	5	58	54
3	10	5	33	36
3	11	5	97	98
3	12	5	103	106
3	13	5	-23	22
3	14	5	59	53
3	15	5	60	62
3	16	5	142	137
3	17	5	33	23
3	18	5	107	85
3	19	5	98	75
3	20	5	114	80
3	0	6	151	156
3	1	6	92	87
3	2	6	83	100
3	3	6	137	124
3	4	6	92	95
3	5	6	176	121
3	6	6	23	21
3	7	6	131	129
3	8	6	72	72
3	9	6	108	107
3	10	6	59	68
3	11	6	67	53
3	12	6	44	43
3	13	6	72	65
3	14	6	50	51
3	15	6	248	174
3	16	6	35	35
3	17	6	36	30
3	18	6	47	46
3	0	7	188	197
3	1	7	58	67
3	2	7	82	77
3	3	7	58	46
3	4	7	40	30
3	5	7	47	45
3	6	7	35	35
3	7	7	69	85
3	8	7	56	49
3	9	7	34	31
3	10	7	51	40
3	11	7	30	33
3	12	7	137	136
3	13	7	35	29
3	14	7	23	24
3	0	8	52	55
3	1	8	35	37
3	2	8	91	130
3	3	8	16	21
3	4	8	49	75
3	5	8	53	59
3	6	8	40	31
3	7	8	43	39
3	8	8	58	40
3	9	8	51	47
4	1	0	84	108
4	2	0	175	168
4	3	0	397	439
4	4	0	128	132
4	5	0	98	86
4	6	0	55	55
4	7	0	154	156
4	8	0	104	94
4	9	0	419	363
4	10	0	259	204
4	11	0	434	397
4	12	0	-21	26
4	13	0	55	39
4	14	0	50	68
4	15	0	319	286
4	16	0	56	43
4	17	0	123	106
4	18	0	75	69
4	19	0	147	119
4	20	0	-24	11
4	21	0	32	27
4	22	0	-20	6
4	23	0	133	120
4	24	0	43	36
4	1	1	131	126
4	2	1	32	42
4	3	1	84	98
4	4	1	392	470
4	5	1	110	135
4	6	1	151	167
4	7	1	61	61
4	8	1	351	334
4	9	1	59	48
4	10	1	209	179
4	11	1	83	54
4	12	1	171	167
4	13	1	136	95
4	14	1	94	79
4	15	1	69	41
4	16	1	201	143
4	17	1	94	65
4	18	1	126	115
4	19	1	35	31
4	20	1	176	174
4	21	1	53	57
4	22	1	127	139
4	23	1	35	30
4	24	1	116	93
4	0	2	133	91
4	1	2	36	42
4	2	2	259	241
4	3	2	199	229
4	4	2	82	88
4	5	2	225	224
4	6	2	221	221
4	7	2	275	265
4	8	2	135	150
4	9	2	204	223
4	10	2	174	174
4	11	2	212	224
4	12	2	32	37
4	13	2	96	92
4	14	2	112	112
4	15	2	195	193
4	16	2	25	35
4	17	2	148	141
4	18	2	50	51
4	19	2	199	167
4	20	2	87	87
4	21	2	30	32
4	22	2	51	52
4	23	2	107	85
4	0	3	319	361
4	1	3	173	214
4	2	3	43	34
4	3	3	151	172
4	4	3	197	237
4	5	3	198	278
4	6	3	43	37
4	7	3	81	86
4	8	3	148	148
4	9	3	294	227
4	10	3	84	79
4	11	3	93	37
4	12	3	167	203
4	13	3	144	135
4	14	3	66	71
4	15	3	81	70
4	16	3	94	84
4	17	3	113	101
4	18	3	24	27
4	19	3	32	36
4	20	3	89	78
4	21	3	105	95
4	22	3	42	42
4	0	4	105	100
4	1	4	103	114
4	2	4	300	321
4	3	4	121	130
4	4	4	115	119
4	5	4	70	67
4	6	4	138	137
4	7	4	67	69
4	8	4	97	109
4	9	4	83	90
4	10	4	224	242
4	11	4	114	119
4	12	4	143	140
4	13	4	63	72
4	14	4	123	115
4	15	4	72	64
4	16	4	114	104
4	17	4	68	68
4	18	4	45	38
4	19	4	90	76
4	20	4	110	95
4	21	4	-15	18
4	22	4	125	97
4	0	5	86	87
4	1	5	173	172
4	2	5	37	44
4	3	5	44	39
4	4	5	74	78
4	5	5	205	216
4	6	5	95	90
4	7	5	162	158
4	8	5	36	43
4	9	5	165	157
4	10	5	56	58
4	11	5	68	61
4	12	5	-25	14
4	13	5	131	141
4	14	5	74	67
4	15	5	78	71
4	16	5	-21	20
4	17	5	108	95
4	18	5	43	46
4	19	5	74	67
4	20	5	31	29
4	0	6	36	38
4	1	6	25	38
4	2	6	182	172
4	3	6	-25	14
4	4	6	113	98
4	5	6	87	81
4	6	6	171	158
4	7	6	35	42
4	8	6	77	74
4	9	6	34	40
4	10	6	139	135
4	11	6	23	21
4	12	6	31	29
4	13	6	46	42
4	14	6	111	101
4	15	6	52	57
4	16	6	55	55
4	17	6	34	33
4	18	6	92	72
4	0	7	41	37
4	1	7	124	121
4	2	7	23	29
4	3	7	33	39
4	4	7	32	26
4	5	7	141	133
4	6	7	31	39
4	7	7	80	85
4	8	7	64	69
4	9	7	56	53
4	10	7	68	77
4	11	7	50	59
4	12	7	56	59
4	13	7	109	94
4	14	7	57	56
4	0	8	-17	2
4	1	8	-17	8
4	2	8	41	43
4	3	8	47	47
4	4	8	-16	14
4	5	8	45	56
4	6	8	82	76
4	7	8	35	27
4	8	8	31	31
4	9	8	69	58
5	1	0	28	23
5	2	0	220	290
5	3	0	-10	19
5	4	0	96	81
5	5	0	188	164
5	6	0	302	349
5	7	0	109	81
5	8	0	23	17
5	9	0	17	19
5	10	0	493	460
5	11	0	-19	21
5	12	0	159	137
5	13	0	53	39
5	14	0	159	137
5	15	0	23	11
5	16	0	112	94
5	17	0	101	68
5	18	0	224	181
5	19	0	47	31
5	20	0	55	35
5	21	0	-21	9
5	22	0	106	74
5	23	0	40	35
5	0	1	31	51
5	1	1	309	441
5	2	1	107	131
5	3	1	342	426
5	4	1	141	163
5	5	1	210	279
5	6	1	96	95
5	7	1	267	311
5	8	1	176	169
5	9	1	331	375
5	10	1	248	224
5	11	1	90	79
5	12	1	114	111
5	13	1	169	153
5	14	1	74	66
5	15	1	67	67
5	16	1	116	103
5	17	1	97	81
5	18	1	58	45
5	19	1	23	25
5	20	1	58	46
5	21	1	198	163
5	22	1	26	24
5	0	2	203	223
5	1	2	173	224
5	2	2	206	264
5	3	2	97	133
5	4	2	52	55
5	5	2	67	68
5	6	2	261	296
5	7	2	17	14
5	8	2	171	145
5	9	2	129	118
5	10	2	285	297
5	11	2	169	171
5	12	2	206	188
5	13	2	131	119
5	14	2	226	202
5	15	2	162	137
5	16	2	107	95
5	17	2	48	41
5	18	2	118	102
5	19	2	133	87
5	20	2	60	62
5	21	2	67	40
5	22	2	77	63
5	23	2	114	81
5	0	3	171	201
5	1	3	113	132
5	2	3	139	170
5	3	3	97	112
5	4	3	157	193
5	5	3	163	171
5	6	3	87	93
5	7	3	178	173
5	8	3	253	249
5	9	3	111	123
5	10	3	31	33
5	11	3	97	89
5	12	3	108	123
5	13	3	133	139
5	14	3	82	82
5	15	3	36	33
5	16	3	138	121
5	17	3	133	133
5	18	3	56	52
5	19	3	33	32
5	20	3	137	131
5	21	3	58	53
5	22	3	63	53
5	0	4	52	83
5	1	4	163	162
5	2	4	78	91
5	3	4	269	277
5	4	4	99	83
5	5	4	219	231
5	6	4	153	156
5	7	4	155	153
5	8	4	167	169
5	9	4	327	331
5	10	4	255	236
5	11	4	133	141
5	12	4	59	63
5	13	4	46	32
5	14	4	-26	23
5	15	4	164	142
5	16	4	22	26
5	17	4	61	51
5	18	4	57	57
5	19	4	108	92
5	20	4	68	63
5	0	5	293	233
5	1	5	98	136
5	2	5	89	131
5	3	5	51	52
5	4	5	129	141
5	5	5	115	123
5	6	5	91	92
5	7	5	137	111
5	8	5	126	133
5	9	5	73	76
5	10	5	66	53
5	11	5	67	93
5	12	5	232	267
5	13	5	32	38
5	14	5	31	39
5	15	5	45	46
5	16	5	111	93
5	17	5	-13	11
5	18	5	63	56
5	19	5	45	63
5	0	6	-24	3
5	1	6	89	72
5	2	6	98	79
5	3	6	145	134
5	4	6	-26	6
5	5	6	113	95
5	6	6	93	78
5	7	6	105	91
5	8	6	98	92
5	9	6	99	99
5	10	6	31	32
5	11	6	143	118
5	12	6	29	33
5	13	6	86	65
5	14	6	26	33
5	15	6	159	139
5	16	6	41	33
5	0	7	112	132
5	1	7	89	78
5	2	7	31	35
5	3	7	43	38
5	4	7	123	186
5	5	7	69	63
5	6	7	45	47
5	7	7	68	67
5	8	7	113	103
5	9	7	45	51
5	10	7	35	33
5	11	7	59	53
5	12	7	126	96
5	13	7	62	51
5	0	8	15	16
5	1	8	45	37
5	2	8	67	61



$x, \quad y, \quad z$ (I)
$x, \quad y, \quad \pm 1+z$ (II, III)
$\frac{1}{2}-x, \quad 1-y, \quad \pm\frac{1}{2}+z$ (IV, V)
$\frac{1}{2}+x, \quad \frac{1}{2}-y, \quad -z$ (VI)
$\frac{1}{2}+x, \quad \frac{1}{2}-y, \quad -1-z$ (VII)
$1-x, \quad -\frac{1}{2}+y, \quad \pm\frac{1}{2}-z$ (VIII, IX)
$1-x, \quad \frac{1}{2}+y, \quad \pm\frac{1}{2}-z$ (X, XI)
$1\frac{1}{2}-x, \quad 1-y, \quad \pm\frac{1}{2}+z$ (XII, XIII)
$-\frac{1}{2}+x, \quad \frac{1}{2}-y, \quad -z$ (XIV)
$-\frac{1}{2}+x, \quad \frac{1}{2}-y, \quad -1-z$ (XV)

In the end 106 intermolecular distances proved to be smaller than 4·20 Å. The smalle stones occur between the carbonyl oxygen atom and other atoms: O(1′)–C(4′), (II–I, I–III) 3·20, O(17)–C(6′), (XI–I, I–IX) 3·35, O(17)–C(2), (VII–I, I–XV) 3·44, O(17)–Br, (X–I, I–VIII) 3·47, O(1′)–C(3′), (II–I, I–III) 3·51 and O(1′)–C(18), (I–IV, V–I) 3·55 Å. The next smallest distance (3·56 Å) is between Br and C(2′) (I–XII, XIII–I). The intermolecular interactions of the type I–XIV and I–VI are rather large (smallest value 3·84 Å). No mutual interactions occur between the Br atoms (see Fig. 4).

Fig. 4. Side and top view of the molecule of APBA. Atoms are indicated with valence radii by overlapping circles. The 'bond-frame' is superposed for reasons of clarity.

All calculations were performed on the IBM 360/50 computer of the Central Computing Laboratory of the University of Leiden. We acknowledge the contributions of Mrs E. W. M. Rutten who wrote the least-

Table 5 (*cont.*)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
5	3	8	53	41	6	0	4	93	106	7	21	0	109	91	7	4	5	149	136	8	0	2	362	434	8	15	6	75	55
5	4	8	36	30	6	1	4	185	206	7	22	0	32	26	7	5	5	144	125	8	1	2	135	155	8	0	7	36	41
5	5	8	77	70	6	2	4	117	139	7	23	0	43	31	7	6	5	91	89	8	2	2	157	159	8	1	7	67	65
5	6	8	74	62	6	3	4	148	137	7	0	1	11	10	7	7	5	158	155	8	3	2	141	148	8	2	7	83	83
6	1	0	152	192	6	4	4	115	123	7	1	1	125	163	7	8	5	125	126	8	4	2	194	217	8	3	7	23	25
6	2	0	40	27	6	5	4	66	67	7	2	1	215	295	7	9	5	113	91	8	5	2	139	155	8	4	7	23	23
6	3	0	55	62	6	6	4	117	129	7	3	1	191	248	7	10	5	-27	15	8	6	2	96	85	8	5	7	68	53
6	4	0	51	56	6	7	4	146	151	7	4	1	96	109	7	11	5	140	130	8	7	2	90	93	8	6	7	99	95
6	5	0	175	149	6	8	4	137	137	7	5	1	157	182	7	12	5	81	74	8	8	2	161	177	8	7	7	37	36
6	6	0	114	109	6	9	4	116	96	7	6	1	303	357	7	13	5	91	83	8	9	2	72	73	8	8	7	63	35
6	7	0	184	201	6	10	4	112	111	7	7	1	101	105	7	14	5	39	33	8	10	2	87	80	8	9	7	42	42
6	8	0	154	135	6	11	4	61	54	7	8	1	78	64	7	15	5	114	84	8	11	2	63	61	8	10	7	133	129
6	9	0	179	159	6	12	4	86	85	7	9	1	177	168	7	16	5	140	107	8	12	2	229	218	8	1	8	30	43
6	10	0	101	97	6	13	4	82	76	7	10	1	181	159	7	17	5	75	64	8	13	2	61	49	8	2	8	-11	19
6	11	0	127	128	6	14	4	137	124	7	11	1	155	131	7	18	5	42	38	8	14	2	36	40	8	3	8	39	56
6	12	0	280	225	6	15	4	34	26	7	12	1	67	60	7	19	5	129	103	8	15	2	67	73	9	1	0	197	225
6	13	0	327	259	6	16	4	85	82	7	13	1	178	157	7	0	6	125	128	8	16	2	139	124	9	2	0	115	117
6	14	0	67	62	6	17	4	53	44	7	14	1	228	234	7	1	6	27	27	8	17	2	97	89	9	3	0	278	271
6	15	0	287	234	6	18	4	111	92	7	15	1	73	54	7	2	6	105	116	8	18	2	92	96	9	4	0	-19	12
6	16	0	270	207	6	19	4	45	43	7	16	1	212	191	7	3	6	22	31	8	19	2	101	97	9	5	0	316	273
6	17	0	77	63	6	20	4	52	48	7	17	1	88	79	7	4	6	144	173	8	20	2	128	123	9	6	0	42	35
6	18	0	43	37	6	21	4	109	79	7	18	1	94	74	7	5	6	60	55	8	21	2	54	59	9	7	0	288	235
6	19	0	262	243	6	0	5	64	72	7	19	1	-21	15	7	6	6	31	25	8	22	2	92	82	9	8	0	226	173
6	20	0	124	107	6	1	5	145	171	7	20	1	63	58	7	7	6	66	56	8	0	3	-20	5	9	9	0	267	208
6	21	0	30	34	6	2	5	110	108	7	21	1	25	31	7	8	6	110	112	8	1	3	117	132	9	10	0	-26	25
6	22	0	92	84	6	3	5	150	162	7	22	1	69	59	7	9	6	29	37	8	2	3	193	213	9	11	0	39	37
6	23	0	181	149	6	4	5	108	117	7	23	1	63	52	7	10	6	28	32	8	3	3	107	110	9	12	0	-28	33
6	24	0	30	19	6	5	5	141	152	7	0	2	91	113	7	11	6	71	67	8	4	3	-21	31	9	13	0	163	139
6	0	1	74	104	6	6	5	133	134	7	1	2	261	323	7	12	6	68	71	8	5	3	112	117	9	14	0	103	91
6	1	1	292	376	6	7	5	79	67	7	2	2	187	216	7	13	6	41	40	8	6	3	181	216	9	15	0	63	64
6	2	1	234	252	6	8	5	-25	27	7	3	2	122	135	7	14	6	40	33	8	7	3	64	62	9	16	0	-33	4
6	3	1	230	241	6	9	5	66	77	7	4	2	179	194	7	15	6	94	79	8	8	3	154	154	9	17	0	169	153
6	4	1	193	212	6	10	5	131	129	7	5	2	208	252	7	16	6	87	69	8	9	3	75	63	9	18	0	88	77
6	5	1	224	223	6	11	5	79	74	7	6	2	182	229	7	0	7	73	65	8	10	3	192	192	9	19	0	-26	11
6	6	1	39	37	6	12	5	63	56	7	7	2	135	147	7	1	7	85	76	8	11	3	47	69	9	20	0	-26	31
6	7	1	67	75	6	13	5	90	85	7	8	2	140	146	7	2	7	53	60	8	12	3	25	24	9	21	0	186	159
6	8	1	178	179	6	14	5	33	80	7	9	2	224	246	7	3	7	84	89	8	13	3	51	48	9	0	1	158	192
6	9	1	246	233	6	15	5	30	29	7	10	2	132	126	7	4	7	74	66	8	14	3	67	69	9	1	1	104	115
6	10	1	127	117	6	16	5	37	39	7	11	2	55	50	7	5	7	88	96	8	15	3	138	129	9	2	1	181	222
6	11	1	177	167	6	17	5	85	80	7	12	2	81	78	7	6	7	31	40	8	16	3	99	83	9	3	1	93	85
6	12	1	203	172	6	18	5	198	113	7	13	2	157	149	7	7	7	69	65	8	17	3	43	41	9	4	1	105	94
6	13	1	155	116	6	0	6	119	113	7	14	2	88	86	7	8	7	45	41	8	18	3	57	80	9	5	1	133	124
6	14	1	91	80	6	1	6	139	145	7	15	2	135	133	7	9	7	67	60	8	19	3	83	79	9	6	1	292	273
6	15	1	112	93	6	2	6	161	170	7	16	2	147	130	7	10	7	-14	3	8	20	3	30	26	9	7	1	64	67
6	16	1	267	231	6	3	6	58	56	7	17	2	123	115	7	11	7	119	92	8	21	3	61	33	9	8	1	53	33
6	17	1	-25	15	6	4	6	-25	18	7	18	2	30	27	7	12	7	65	50	8	0	4	111	123	9	9	1	35	35
6	18	1	-25	37	6	5	6	60	50	7	19	2	69	64	7	0	8	66	74	8	1	4	141	147	9	10	1	271	257
6	19	1	196	166	6	6	6	144	134	7	20	2	79	77	7	1	8	48	51	8	2	4	129	119	9	11	1	77	72
6	20	1	178	142	6	7	6	34	39	7	21	2	116	87	7	2	8	53	64	8	3	4	140	139	9	12	1	162	132
6	21	1	54	58	6	8	6	-24	20	7	22	2	94	80	7	3	8	-12	11	8	4	4	192	195	9	13	1	47	65
6	22	1	107	103	6	9	6	101	86	7	23	2	37	31	7	4	8	69	73	8	5	4	352	371	9	14	1	138	137
6	23	1	70	64	6	10	6	111	102	7	0	3	123	143	7	5	8	46	51	8	6	4	73	80	9	15	1	-33	15
6	24	1	23	26	6	11	6	48	51	7	1	3	110	114	7	6	8	22	13	8	7	4	139	152	9	16	1	133	125
6	0	2	64	77	6	12	6	29	30	7	2	3	252	293	8	1	0	119	119	8	8	4	142	136	9	17	1	59	31
6	1	2	260	293	6	13	6	51	46	7	3	3	50	44	8	2	0	-12	8	8	9	4	161	163	9	18	1	191	152
6	2	2	453	569	6	14	6	65	63	7	4	3	132	153	8	3	0	117	117	8	10	4	25	29	9	19	1	36	49
6	3	2	210	275	6	15	6	39	41	7	5	3	135	143	8	4	0	264	307	8	11	4	43	38	9	20	1	50	73
6	4	2	225	234	6	16	6	43	48	7	6	3	175	215	8	5	0	-16	13	8	12	4	87	72	9	21	1	71	66
6	5	2	187	186	6	17	6	39	32	7	7	3	174	178	8	6	0	41	31	8	13	4	135	133	9	22	1	41	63
6	6	2	160	185	6	0	7	-22	4	7	8	3	116	121	8	7	0	97	88	8	14	4	68	57	9	0	2	195	229
6	7	2	143	152	6	1	7	31	27	7	9	3	158	183	8	8	0	198	204	8	15	4	43	57	9	1	2	167	199
6	8	2	150	164	6	2	7	92	87	7	10	3	150	155	8	9	0	77	59	8	16	4	53	56	9	2	2	99	97
6	9	2	78	75	6	3	7	53	52	7	11	3	166	156	8	10	0	-22	1	8	17	4	153	127	9	3	2	157	176
6	10	2	97	100	6	4	7	21	25	7	12	3	90	82	8	11	0	-23	13	8	18	4	45	34	9	4	2	102	102
6	11	2	88	86	6	5	7	111	114	7	13	3	131	123	8	12	0	197	234	8	19	4	62	69	9	5	2	175	150
6	12	2	80	77	6	6	7	67	57	7	14	3	136	117	8	13	0	71	55	8	20	4	48	34	9	6	2	71	72
6	13	2	183	162	6	7	7	20	19	7	15	3	142	119	8	14	0	44	32	8	0	5	142	159	9	7	2	142	147
6	14	2	130	117	6	8	7	27	26	7	16	3	80	69	8	15	0	-25	15	8	1	5	82	85	9	8	2	107	121
6	15	2	157	135	6	9	7	48	50	7	17	3	47	35	8	16	0	160	146	8	2	5	149	166	9	9	2	135	155
6	16	2	217	172	6	10	7	84	74	7	18	3	55	62	8	17	0	66	60	8	3	5	94	99	9	10	2	72	53
6	17	2	35	29	6	11	7	45	38	7	19	3	101	87	8	18	0	88	77	8	4	5	103	108	9	11	2	86	82
6	18	2	-24	21	6	12	7	102	84	7	20	3	37	34	8	19	0	98	87	8	5	5	69	57	9	12	2	188	177
6	19	2	116	107	6	13	7	61	53	7	21	3	24	21	8	20	0	113	126	8	6	5	175	169	9	13	2	158	141
6	20	2	88	66	6	0	8	22	23	7	22	3	76	57	8	21	0	53	52	8	7	5	154	154	9	14	2	153	123
6	21	2	39	32	6	1	8	50	54	7	0	4	112	119	8	22	0	58	51	8	8	5	63	54	9	15	2	97	77
6	22	2	71	56	6	2	8	49	55	7	1	4	158	186	8	23	0	37	33	8	9	5	44	42	9	16	2	132	111
6	23	2	81	73	6	3	8	33	38	7	2	4	103	109	8	0	1	78	66	8	10	5	173	170	9	17	2	109	92
6	0	3	267	304	6	4	8	35	28	7	3	4	71	64	8	1	1	186	243	8	11	5	34	35	9	18	2	63	65
6	1	3	215	244	6	5	8	48	54	7	4	4	184	188	8	2	1	138	155	8	12	5	77	79	9	19	2	-24	23
6	2	3	137	153	6	6	8	40	43	7	5	4	215	226	8	3	1	229	255	8	13	5	37	39	9	20	2	81	57
6	3	3	81	94	7	1	0	176	241	7	6	4	151	160	8	4	1	73	69	8	14	5	118	106	9	21	2	53	51
6	4	3	305	322	7	2	0	177	209	7	7	4	145	148	8	5	1	186	188	8	15	5	-20	8	9	22	2	52	55
6	5	3	190	207	7	3	0	141	133	7	8	4	147	140	8	6	1	113	108	8	16	5	73	61	9	0	3	43	61
6	6	3	85	89	7	4	0	153	144	7	9	4	135	176	8	7	1	276	268	8	17	5	39	25	9	1	3	178	176
6	7	3	51	67	7	5	0	225	258	7	10	4	104	94	8	8	1	-20	5	8	18	5	63	54	9	2	3	115	107
6	8	3	128	149	7	6	0	144	169	7	11	4	107	94	8	9	1	169	145	8	0	6	-25	14	9	3	3	161	173
6	9	3	158	144	7	7	0	104	105	7	12	4	125	135	8	10	1	101	73	8	1	6	56	40	9	4	3	37	33
6	10	3	93	97	7	8	0	56	51	7	13	4	120	100	8	11	1	201	191	8	2	6	43	31	9	5	3	77	73
6	11	3	148	156	7	9	0	259	226	7	14	4	31	28	8	12	1	157	174	8	3	6	107	93	9	6	3	147	157
6	12	3	106	97	7	10	0	92	91	7	15	4	50	53	8	13	1	192	195	8	4	6	24	21	9	7	3	91	79
6	13	3	157	153	7	11	0	142	129	7	16	4	198	96	8	14	1	87	81	8	5	6	113	107	9	8	3	78	91
6	14	3	93	83	7	12	0	61	32	7	17	4	27	25	8	15	1	264	256	8	6	6	48	40	9	9	3	133	119
6	15	3	53	46	7	13	0	227	221	7	18	4	76	65	8	16	1	162	137	8	7	6	76	72	9	10	3	187	213
6	16	3	107	91	7	14	0	150	142	7	19	4	70	56	8	17	1	36	36	8	8	6	-23	21	9	11	3	135	123
6	17	3	93	76	7	15	0	110	74	7	20	4	71	59	8	18	1	60	53	8	9	6	68	71	9	12	3	43	31
6	18	3	73	60	7	16	0	45	37	7	21	4	58	54	8	19	1	82	100	8	10	6	37	39	9	13	3	47	57
6	19	3	116	99	7	17	0	184	180	7	0	5	124	137	8	20	1	30	23	8	11	6	67	66	9	14	3	165	123
6	20	3	58	52	7	18	0	102	86	7	1	5	84	79	8	21	1	-19	20	8	12	6	80	77	9	15	3	136	112
6	21	3	68	63	7	19	0	64	57	7	2	5	22	22	8	22	1	33	30	8	13	6	94	83	9	16	3	-27	33
6	22	3	60	52	7	20	0	-20	6	7	3	5	44	73	8	23	1	-12	98	8	14	6	-16	12	9	17	3	-25	44
9	18	3	122	109	9	9	4	30	29	9	0	5	30	39	9	11	5	116	131	9	4	6	87	91	9	2	7	37	53
9	19	3	139	103	9	10	4	43	55	9	1	5	126	128	9	12	5	38	26	9	5	6	56	59	9	3	7	72	85
9	0	4	231	258	9	11	4	-30	31	9	2	5	70	77	9	13	5	98	100	9	6	6	39	65	9	4	7	55	67
9	1	4	66	64	9	12	4	133	122	9	3	5	154	168	9	14	5	-23	20	9	7	6	-27	26	9	5	7	75	87
9	2	4	28	40	9	13	4	-29	32	9	4	5	108	131	9	15	5	175	130	9	8	6	93	109	9	6	7	72	47
9	3	4	99	103	9	14	4	100	92	9	5	5	60	69	9	16	5	-19	25	9	9	6	-25	3	9	7	7	55	59
9	4	4	121	117	9	15	4	37	43	9	6	5	108	131	9	17	5	65	56	9	10	6	34	44	9	8	7	-18	8
9	5	4	41	56	9	16	4	62	42	9	7	5	95	83	9	0	6	174	192	9	11	6	-22	30	9	9	7	41	53
9	6	4	63	73	9	17	4	-22	42	9	8	5	-29	20	9	1	6	58	56	9	12	6	159	134					
9	7	4	118	116	9	18	4	107	78	9	9	5	135	96	9	2	6	40	52	9	0	7	33	59					
9	8	4	129	118	9	19	4	33	32	9	10	5	57	66	9	3	6	49	63	9	1	7	33	55					

squares and Fourier programs and of R. A. G. de Graaff for developing the geometry programs. We wish to express our thanks to Mrs L. Willemsen, who produced the photographs and to F. C. Mijlhoff for discussions on the *R*-ratio test.

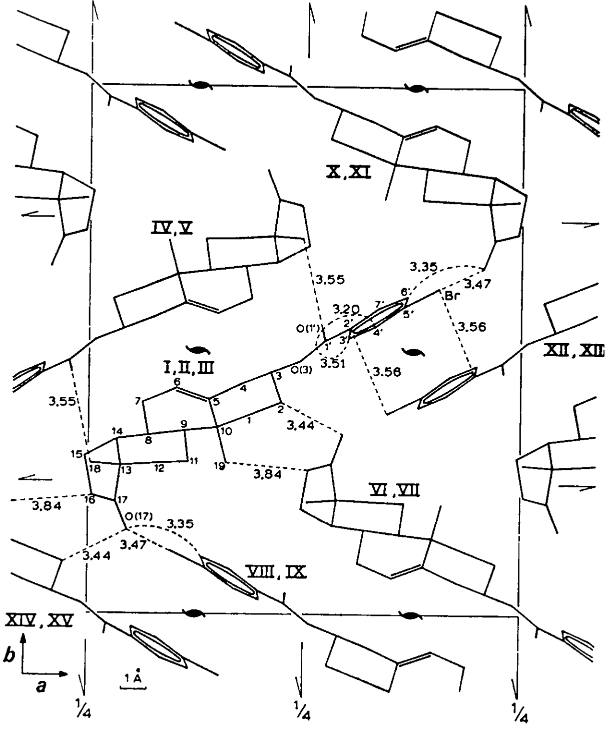


Fig. 5. Projection of APBA along [001]. The Roman numbers are explained in the text. Dotted lines indicate intermolecular distances. The reference molecule I is obtained by application of the transformation $\frac{1}{2}+x$, $\frac{1}{2}-y$, $\bar{z}$ to the coordinates of Table 2 (column 'simultaneous').

References

Altona, C. (1964). *Acta Cryst.* **17**, 1282.

Altona, C., Geise, H. J. & Romers, C. (1968). *Tetrahedron*, **24**, 13.

Bots, J. P. L. (1958). *Rec. Trav. Chim. Pays-Bas*, **77**, 1010.

Braun, P. B., Hornstra, J. & Leenhouts, J. I. (1969). *Philips Res. Repts.* **24**, 427.

Bucourt, R. (1964). *Bull. Soc. Chim. France*, p. 2080.

Bucourt, R. & Hainaut, D. (1965). *Bull. Soc. Chim. France*, p. 1366.

Cromer, D. T. & Waber, J. T. (1965). *Acta Cryst.* **18**, 104.

Geise, H. J., Altona, C. & Romers, C. (1967). *Tetrahedron*, **23**, 439.

Hamilton, W. C. (1964). In *Statistics in Physical Science*. New York: Ronald Press.

Hamilton, W. C. (1965). *Acta Cryst.* **18**, 502.

Hesper, B., Geise, H. J. & Romers, C. (1969). *Rec. Trav. Chim. Pays-Bas*, **88**, 871.

Hoog, A. J. de & Havinga, E. (1970). *Rec. Trav. Chim. Pays-Bas*. In the press.

International Tables for X-ray Crystallography (1962). Vol. III, p. 202. Birmingham: Kynoch Press.

IUPAC – IUB 1967 *Revised Tentative Rules for Steroid Nomenclature* (1969). *Biochem. J.* **113**, 5; *Steroids*, **13**, 278.

Karle, I. L. & Karle, J. (1969). *Acta Cryst.* B**25**, 434.

Kok, A. J. de & Romers, C. (1969). *Rec. Trav. Chim. Pays-Bas*, **88**, 625.

Phillips, D. C. (1956). *Acta Cryst.* **9**, 819.

Portheine, J. C., Romers, C. & Rutten, E. W. M. (1970). To be published.

Pot, J. (1964). Thesis, University of Leiden, p. 26.

Rae, A. D. (1965). *Acta Cryst.* **19**, 683.

Stewart, R. F., Davidson, E. R. & Simpson, W. T. (1965). *J. Chem. Phys.* **42**, 3175.

Vledder, H. J., Mijlhoff, F. C., Leyte, J. C. & Romers, C. (1970). *J. Mol. Struct.* In the press.