References

Abrahamsson, S. (1959). *Ark. Kemi*, **14**, 65.

Abrahamsson, S. & Ryderstedt-Nahringbauer, I. (1962). *Acta Cryst.* **15**, 1261.

Abrahamsson, S., Ställberg-Stenhagen, S. & Stenhagen, E. (1962). *Progress in the Chemistry of Fats and Other Lipids*, Volume 7. Oxford: Pergamon Press.

Abrahamsson, S., Hodgkin, D. C. & Maslen, E. N. (1962). *Biochem. J.* In the press.

Abrahamsson, S. & Maslen, E. (1962). *Z. Kristallogr.* In the press.

Ahmed, F. R. & Cruickshank, D. W. J. (1953). *Acta Cryst.* **6**, 385.

Aleby, S. (1962). *Acta Cryst.* **15**, 1248.

Berghuis, J., Haanappel, IJ. M., Potters, M., Loopstra, B. O., MacGillavry, C. H. & Veenendaal, A. L. (1955). *Acta Cryst.* **8**, 478.

Craven, B. & Jeffrey, G. A. (1959). *Nature, Lond.* **183**, 676.

Darlow, S. F. (1960). *Acta Cryst.* **13**, 683.

Kay, M. I. & Katz, L. (1958). *Acta Cryst.* **11**, 289.

Kitaigorodskii, A. I. (1957). *Kristallografiya*, **2**, 646.

Larsson, K. (1962). *Acta Chem. Scand.* In the press.

McWeeny, R. (1952). *Acta Cryst.* **5**, 463.

Mills, O. S. & Rollett, J. S. (1961). *Computing Methods and the Phase Problem in X-ray Crystal Analysis*, p. 107. London: Pergamon Press.

Smith, B. & Hernestam, S. (1954). *Acta Chem. Scand.* **8**, 1111.

Viervoll, H. & Øgrim, O. (1949). *Acta Cryst.* **2**, 277.

Acta Cryst. (1963). **16**, 409

A Direct Determination of the Molecular Structure of Prostaglandin F_{2-1}

By Sixten Abrahamsson

Crystallography Group, Institute of Medical Biochemistry, University of Göteborg, Sweden

(*Received* 9 *July* 1962)

The tri-*p*-bromobenzoate of the methyl ester of prostaglandin $F_{2-1}(C_{42}H_{47}O_8Br_3)$ is orthorhombic with $a = 26{\cdot}14$, $b = 33{\cdot}93$ and $c = 4{\cdot}76$ Å. The space group is $P2_12_12_1$ with $Z = 4$. The structure was solved by heavy-atom methods and refined by three-dimensional anisotropic least-squares treatment to give the molecular structure and configuration of prostaglandin F_{2-1}, which belongs to a new class of hormones having smooth-muscle-stimulating and blood-pressure-depressing activity.

Introduction

A smooth-muscle-stimulating and blood-pressure-depressing activity was discovered in human semen by Goldblatt (1933) and by von Euler (1934, 1935) who also found a similar activity in sheep sperm and named the factor 'prostaglandin'.

In 1960 Bergström & Sjövall (1960) isolated two active crystalline compounds $PGE_1(C_{20}H_{34}O_5)$ and $PGF_{1-1}(C_{20}H_{36}O_5)$ from sheep prostate glands. Reduction of PGE_1 with borohydride (Bergström *et al.*, 1962) yielded PGF_{1-1} together with the isomeric compound PGF_{2-1}.

The tri-*p*-bromo- and tri-*p*-iodobenzoates of the methyl ester of PGF_{2-1} were prepared by Prof. S. Bergström who kindly provided them for an X-ray analysis in order to determine *ab initio* the molecular structures.

Experimental

The two benzoates crystallize as beautiful needles from ethanol. All crystals studied gave excellent X-ray photographs, which indicated that the two derivatives are isomorphous. The unit cell is orthorhombic with space group $P2_12_12_1$. The cell dimensions are:

	a	*b*	*c*
Br-derivative	26·14 Å	33·93 Å	4·76 Å
I-derivative	26·49	34·39	4·76

Full three-dimensional data (Cu $K\alpha$ radiation) were collected for the bromo compound. Multiple-film Weissenberg photographs were recorded for the 0–2 layers about *c* (needle direction) and the 0–5 layers about *a*. Only *hk*0 intensities were estimated for the iodo derivative. The intensities were corrected for the Lorentz and polarization factors but not for absorption.

Structure determination

The initial work was done on the (001) projection. From a sharpened Patterson projection of the I-derivative, the relative positions of the heavy atoms of the four molecules per cell were obtained by simple vector addition and subtraction. The origin was then determined from the known symmetry of the projection. As expected the Patterson synthesis was completely dominated by I–I vectors (Fig. 1).

An electron-density projection showed most of the atoms of the molecule (Fig. 2) but also contained some spurious detail. This, however, was still present, when more atoms, *e.g.* those of the benzoate groups were included in the analysis and the general appearance of the maps did not improve much from that of Fig. 2. Similar effects were encountered with the Br-derivative $hk0$ data. They were caused by the large anisotropic vibrations of the heavy atoms. As soon as these were accounted for a projection could be found which was chemically sensible and which did refine. Anisotropic least-squares treatment of the Br-derivative projection data reduced R to 20%.

At that stage the three-dimensional data (1776 independent reflexions) were available. A Patterson synthesis sharpened to point atoms at rest (Abrahamsson & Maslen, 1963) was calculated. The resolution in the c-direction was still low due to the lack of high orders of l. This, and the presence of mirror planes, caused some trouble in finding the z-coordinates of the heavy atoms (see Fig. 3). Coordinates chosen to give the best compromise solution to the Patterson later proved to be surprisingly accurate (within 0·17 Å).

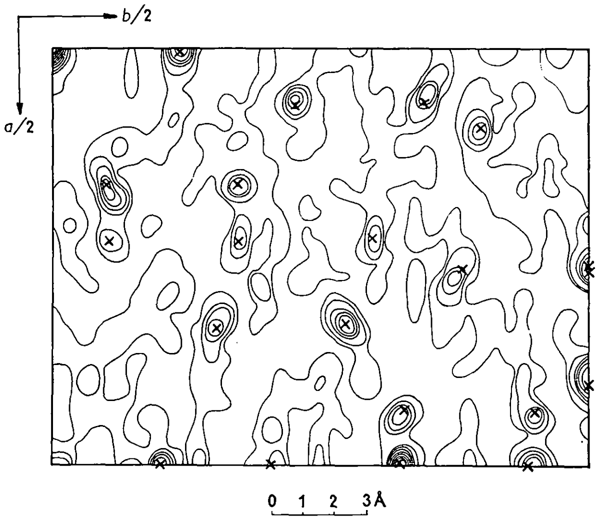


Fig. 1. Patterson (001) projection for the I-derivative. Crosses mark heavy atom vectors calculated from the final bromine positions.

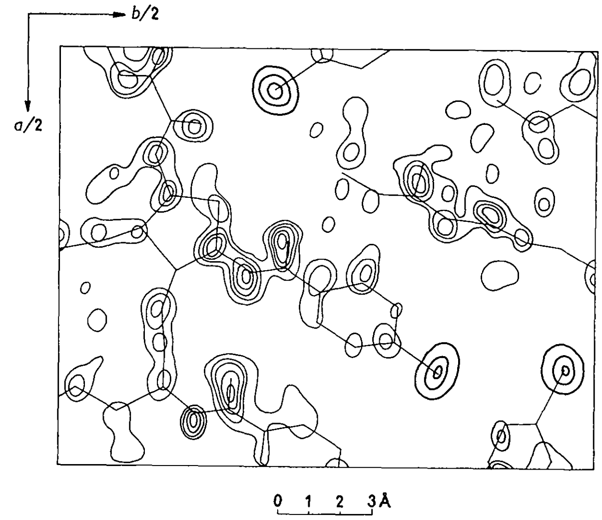


Fig. 2. Iodine-phased electron density projection along the c-axis with the correct structure outlined. Contours at arbitrary but equal levels except for the heavy atom, which has different contour intervals.

Table 1. *Atomic coordinates*

	x/a	y/b	z/c
Br_1	0·63174	0·47212	0·01758
Br_2	0·63476	0·35299	−0·21371
Br_3	0·29836	0·19886	0·16054
O_1	0·34242	0·12472	−0·51624
O_2	0·37917	0·08772	−0·17795
O_3	0·51648	0·17763	−0·03904
O_4	0·47548	0·21145	0·27676
O_5	0·39422	0·33494	−0·06161
O_6	0·42681	0·29515	−0·37597
O_7	0·64002	0·16036	0·40039
O_8	0·68815	0·12388	0·11804
C_1	0·19407	0·05198	−0·11009
C_2	0·19771	0·08252	−0·28724
C_3	0·24290	0·09588	−0·37575
C_4	0·28700	0·08330	−0·24648
C_5	0·28642	0·05488	−0·04880
C_6	0·23859	0·03885	0·02603
C_7	0·33866	0·10228	−0·32869
C_8	0·42725	0·10450	−0·23528
C_9	0·43282	0·14464	−0·10760
C_{10}	0·48675	0·14279	0·04589
C_{11}	0·51282	0·10674	−0·10328
C_{12}	0·46710	0·07703	−0·12347
C_{13}	0·50569	0·20957	0·10708
C_{14}	0·54020	0·24402	0·02812
C_{15}	0·52861	0·28079	0·12427
C_{16}	0·55678	0·31405	0·10016
C_{17}	0·59564	0·30890	−0·10939
C_{18}	0·60688	0·27266	−0·24344
C_{19}	0·57848	0·23938	−0·15468
C_{20}	0·47724	0·03968	−0·28187
C_{21}	0·49046	0·00396	−0·08600
C_{22}	0·49111	0·47002	−0·23930
C_{23}	0·48345	0·43217	−0·40866
C_{24}	0·45817	0·39924	−0·22800
C_{25}	0·45393	0·36086	−0·41734
C_{26}	0·42221	0·33257	−0·23383
C_{27}	0·39942	0·26075	−0·25072
C_{28}	0·55798	0·09409	0·09676
C_{29}	0·60572	0·09796	−0·01240
C_{30}	0·65203	0·09038	0·15999
C_{31}	0·67528	0·15801	0·24266
C_{32}	0·70630	0·19000	0·13500
C_{33}	0·69792	0·22707	0·24057
C_{34}	0·72300	0·26250	0·14650
C_{35}	0·76164	0·25635	−0·03000
C_{36}	0·77360	0·21976	−0·14132
C_{37}	0·74627	0·18892	−0·03900
C_{38}	0·68358	0·05368	0·07943
C_{39}	0·65506	0·01565	0·14440
C_{40}	0·31319	0·47755	−0·56601
C_{41}	0·33840	0·44075	−0·64926
C_{42}	0·30974	0·40358	−0·57723

Table 2. *Vibrational parameters*

Allowance was made for anisotropic vibrations with $2^{-(h^2b_{11}+k^2b_{22}+l^2b_{33}+klb_{23}+hlb_{13}+hkb_{12})}$

	b_{11}	b_{22}	b_{33}	b_{23}	b_{13}	b_{12}
Br_1	0·00293	0·00392	0·29367	−0·00325	−0·01480	0·00287
Br_2	0·00878	0·00236	0·28466	0·00437	0·00991	−0·00608
Br_3	0·00431	0·00167	0·24959	0·00221	0·00609	0·00184
O_1	0·00262	0·00154	0·16485	0·00902	0·00414	0·00097
O_2	0·00241	0·00158	0·04023	0·00450	−0·00858	−0·00018
O_3	0·00208	0·00095	0·10525	−0·00587	0·00649	−0·00086
O_4	0·00521	0·00114	0·19606	−0·00059	0·00333	−0·00070
O_5	0·00409	0·00170	0·15280	0·00683	0·00976	−0·00251
O_6	0·00555	0·00149	0·17847	0·00366	0·00426	0·00074
O_7	0·00406	0·00239	0·23268	−0·00167	0·01554	−0·00369
O_8	0·00220	0·00206	0·03925	0·00169	0·00254	−0·00108
C_1	0·00474	0·00172	0·18647	−0·00406	0·02437	−0·00206
C_2	0·00161	0·00347	0·23723	−0·00858	−0·00886	−0·00059
C_3	0·00329	0·00218	0·33806	0·00369	−0·00505	0·00178
C_4	0·00345	0·00130	0·26335	−0·01230	−0·00462	−0·00110
C_5	0·00294	0·00164	0·26255	−0·00572	−0·01158	−0·00188
C_6	0·00263	0·00317	0·21271	0·01304	0·00274	−0·00199
C_7	0·00197	0·00134	0·17372	0·01241	−0·00242	−0·00137
C_8	0·00120	0·00103	0·08023	0·00371	0·01110	−0·00080
C_9	0·00295	0·00093	0·14333	−0·00480	0·00034	−0·00115
C_{10}	0·00185	0·00093	0·13316	−0·00518	0·00568	−0·00108
C_{11}	0·00139	0·00074	0·20162	0·00628	0·00733	−0·00072
C_{12}	0·00190	0·00081	0·17588	−0·01310	−0·00329	0·00010
C_{13}	0·00338	0·00106	0·21594	0·00536	0·00169	0·00104
C_{14}	0·00310	0·00135	0·07704	−0·00545	0·00767	−0·00304
C_{15}	0·00427	0·00115	0·30794	0·00247	0·00390	−0·00095
C_{16}	0·00502	0·00186	0·06394	−0·00083	−0·00206	−0·00248
C_{17}	0·00639	0·00152	0·19506	0·01874	0·01861	−0·00129
C_{18}	0·00512	0·00105	0·23684	−0·00604	0·01575	−0·00250
C_{19}	0·00514	0·00081	0·22429	−0·00166	0·04025	−0·00079
C_{20}	0·00287	0·00084	0·13278	0·00140	−0·01379	−0·00038
C_{21}	0·00334	0·00090	0·24077	−0·00104	−0·02731	0·00151
C_{22}	0·00400	0·00062	0·11502	−0·00293	−0·00679	0·00049
C_{23}	0·00304	0·00106	0·12249	−0·00260	−0·00228	−0·00114
C_{24}	0·00356	0·00119	0·12110	−0·01377	−0·01040	−0·00047
C_{25}	0·00341	0·00038	0·26662	0·00114	0·00778	−0·00088
C_{26}	0·00276	0·00102	0·08223	−0·00112	0·01062	0·00041
C_{27}	0·00396	0·00096	0·20239	0·00053	0·01334	−0·00261
C_{28}	0·00246	0·00022	0·15666	0·00024	−0·00348	−0·00004
C_{29}	0·00212	0·00092	0·19003	0·00467	0·01987	−0·00008
C_{30}	0·00240	0·00057	0·15615	−0·00493	−0·00688	−0·00004
C_{31}	0·00252	0·00094	0·20924	0·00691	−0·02245	−0·00128
C_{32}	0·00331	0·00140	0·14783	0·00240	0·01644	−0·00053
C_{33}	0·00487	0·00236	0·28037	−0·00400	0·02831	−0·00182
C_{34}	0·00581	0·00106	0·26741	0·01266	0·03284	−0·00085
C_{35}	0·00363	0·00038	0·25971	−0·00464	0·00824	−0·00082
C_{36}	0·00336	0·00146	0·28297	−0·00609	0·01990	−0·00405
C_{37}	0·00273	0·00185	0·32248	−0·00107	0·02743	0·00014
C_{38}	0·00345	0·00120	0·10454	0·00545	−0·01850	−0·00076
C_{39}	0·00400	0·00033	0·19997	−0·00638	0·02130	0·00032
C_{40}	0·00261	0·00021	0·19404	−0·00685	−0·02013	0·00009
C_{41}	0·00350	0·00129	0·21235	−0·00036	0·00382	0·00145
C_{42}	0·00468	0·00113	0·20270	0·00345	−0·02783	−0·00103

The three-dimensional electron-density series calculated on the bromine phases showed the complete molecule as found from the (001) projection. Two rounds of Fourier refinement, during which least-squares methods were applied to the heavy atoms, reduced R to 23% for all observed reflexions and confirmed the assignment of atomic numbers to the peaks in the projection analysis.

All atoms were finally included in the anisotropic least-squares refinement. Three cycles reduced R to 10·9%. It was not considered worth while to perform further 7-hour least-squares cycles as the molecular structure is fully established with the accuracy in positions reached. However, the shifts in the least accurately placed atoms (the benzene-ring carbons) approached the standard deviations.

For carbon and oxygen the scattering curves of Berghuis *et al.* (1955) were used and for bromine that of Thomas & Umeda (1957) corrected for the f' component of the anomalous dispersion (Dauben & Templeton, 1955). The calculations were performed on a Ferranti-Mercury computer with programs described by Mills & Rollett (1961). The weighting scheme adopted in the least-squares refinement was

Table 3. *Interatomic distances and bond angles*

Bond distances

Bond		Bond	
Br_1–C_1	1·88 Å	C_{33}–C_{34}	1·44 Å
Br_2–C_{17}	1·88	C_{34}–C_{35}	1·33
Br_3–C_{35}	1·90	C_{35}–C_{36}	1·39
C_1–C_2	1·34	C_{36}–C_{37}	1·36
C_2–C_3	1·33	C_{37}–C_{32}	1·33
C_3–C_4	1·37	C_8–C_9	1·50
C_4–C_5	1·35	C_9–C_{10}	1·59
C_5–C_6	1·41	C_{10}–C_{11}	1·57
C_1–C_6	1·40	C_{11}–C_{12}	1·57
C_4–C_7	1·55	C_{12}–C_{20}	1·50
C_7–O_1	1·18	C_{20}–C_{21}	1·58
C_7–O_2	1·37	C_{21}–C_{22}	1·52
O_2–C_8	1·41	C_{22}–C_{23}	1·53
C_{10}–O_3	1·47	C_{23}–C_{24}	1·56
O_3–C_{13}	1·32	C_{24}–C_{25}	1·59
C_{13}–O_4	1·13	C_{25}–C_{26}	1·54
C_{13}–C_{14}	1·52	C_{26}–O_5	1·10
C_{14}–C_{15}	1·36	C_{26}–O_6	1·44
C_{15}–C_{16}	1·35	O_6–C_{27}	1·49
C_{16}–C_{17}	1·43	C_{11}–C_{28}	1·58
C_{17}–C_{18}	1·42	C_{28}–C_{29}	1·36
C_{18}–C_{19}	1·42	C_{29}–C_{30}	1·48
C_{14}–C_{19}	1·34	C_{30}–C_{38}	1·54
C_{30}–O_8	1·49	C_{38}–C_{39}	1·52
O_8–C_{31}	1·34	C_{39}–C_{40}	1·58
O_7–C_{31}	1·19	C_{40}–C_{41}	1·47
C_{31}–C_{32}	1·45	C_{41}–C_{42}	1·51
C_{32}–C_{33}	1·37		

Bond angles

Bond angle		Bond angle		Bond angle	
Br_1–C_1–C_2	123°	C_{18}–C_{17}–Br_2	117°	C_{10}–C_{11}–C_{28}	105°
Br_1–C_1–C_6	118	C_{17}–C_{18}–C_{19}	117	C_{12}–C_{11}–C_{28}	116
C_6–C_1–C_2	118	C_{18}–C_{19}–C_{14}	120	C_{11}–C_{12}–C_8	99
C_1–C_2–C_3	122	C_{30}–O_8–C_{31}	116	C_{11}–C_{12}–C_{20}	116
C_2–C_3–C_4	120	O_8–C_{31}–O_7	122	C_8–C_{12}–C_{20}	118
C_3–C_4–C_5	122	O_8–C_{31}–C_{32}	110	C_{12}–C_{20}–C_{21}	112
C_2–C_4–C_3	119	O_7–C_{31}–C_{32}	127	C_{20}–C_{21}–C_{22}	108
C_2–C_4–C_5	119	C_{31}–C_{32}–C_{33}	118	C_{21}–C_{22}–C_{23}	112
C_4–C_5–C_6	118	C_{31}–C_{32}–C_{37}	130	C_{22}–C_{23}–C_{24}	112
C_5–C_6–C_1	120	C_{37}–C_{32}–C_{33}	112	C_{23}–C_{24}–C_{25}	108
O_1–C_7–C_4	122	C_{32}–C_{33}–C_{34}	125	C_{24}–C_{25}–C_{26}	103
O_2–C_7–C_4	113	C_{33}–C_{34}–C_{35}	114	C_{25}–C_{26}–O_5	137
O_1–C_7–O_2	124	C_{34}–C_{35}–C_{36}	124	C_{25}–C_{26}–O_6	104
C_7–O_2–C_8	116	C_{34}–C_{35}–Br_3	118	O_5–C_{26}–O_6	118
C_{10}–O_3–C_{13}	114	C_{36}–C_{35}–Br_3	119	C_{26}–O_6–C_{27}	117
O_3–C_{13}–O_4	125	C_{35}–C_{36}–C_{37}	116	C_{11}–C_{28}–C_{29}	116
O_3–C_{13}–C_{14}	112	C_{36}–C_{37}–C_{32}	128	C_{28}–C_{29}–C_{30}	121
O_4–C_{13}–C_{14}	123	C_{12}–C_8–C_9	111	C_{29}–C_{30}–C_{38}	116
C_{13}–C_{14}–C_{15}	119	O_2–C_8–C_9	112	C_{29}–C_{30}–O_8	108
C_{13}–C_{14}–C_{19}	120	O_2–C_8–C_{12}	108	O_8–C_{30}–C_{38}	104
C_{19}–C_{14}–C_{15}	121	C_8–C_9–C_{10}	104	C_{30}–C_{38}–C_{39}	112
C_{14}–C_{15}–C_{16}	128	C_9–C_{10}–C_{11}	102	C_{38}–C_{39}–C_{40}	113
C_{15}–C_{16}–C_{17}	110	C_9–C_{10}–O_3	108	C_{39}–C_{40}–C_{41}	113
C_{16}–C_{17}–C_{18}	124	C_{11}–C_{10}–O_3	106	C_{40}–C_{41}–C_{42}	115
C_{16}–C_{17}–Br_2	118	C_{10}–C_{11}–C_{12}	101		

$$w = \frac{1}{1+[(|F_o|-8|F_{\mathrm{min.}}|)/5|F_{\mathrm{min.}}|]^2}\,.$$

Discussion

The coordinates of the atoms in the molecule other than hydrogen are given in Table 1, the vibrational parameters in Table 2. The final structure factors are listed in Table 6. A composite drawing of the three-dimensional electron-density series based on the final phases is shown in Fig. 4.

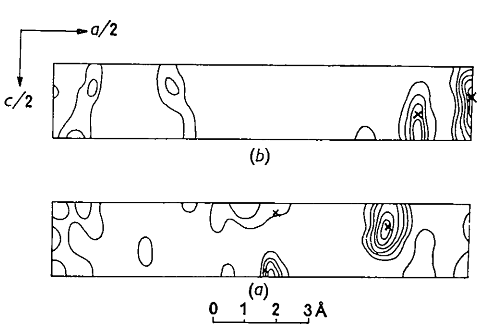


Fig. 3. Sections of the three-dimensional point atoms at rest. Patterson synthesis for the bromo derivative. (*a*) Harker section at $z=1/2$, (*b*) section at $z=26/80$. Crosses mark Br–Br vectors calculated from the final positions.

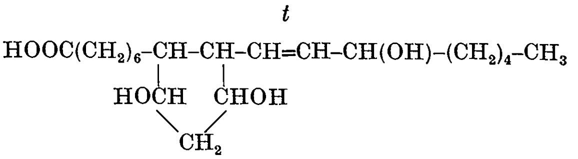
Table 4. *Average values for different classes of bond distances and angles*

	Bond		Angle
Benzene rings	C – C	1·38 ± 0·05 Å	120 ± 10°
Unstrained carbon single bonds	C – C	1·54 ± 0·07	111 ± 8
Carboxyl carbon to oxygen	C = O C – O	1·15 ± 0·05 1·37 ± 0·07	
Other carbon–oxygen	C – O	1·46 ± 0·05	
	Br – C	1·89 ± 0·01	

Table 5. *Some short contacts between one molecule and its equivalent repeated along the c-axis*

O_1–O_2	3·52 Å	C_{15}–C_{18}	3·64 Å
O_3–O_4	3·62	C_{15}–C_{19}	3·93
O_7–O_8	3·84	C_{16}–C_{18}	3·67
O_5–O_6	3·63	C_{33}–C_{36}	3·55
C_2–C_6	3·74	C_{33}–C_{37}	3·88
C_3–C_5	3·67	C_{34}–C_{36}	3·92
C_3–C_6	3·44	C_8–C_{10}	3·98

The molecular structure of the tri-*p*-bromobenzoate derivative of the methyl ester of $PGF_{2-1}(C_{42}H_{47}O_8Br_3)$ is all in accordance with the formula (I) for the free acid of PGF_{2-1} independently arrived at by Bergström *et al.* (1962*a*) using chemical and physicochemical methods other than X-ray diffraction.



$$\mathrm{HOOC(CH_2)_6\text{-}\underset{HOCH}{CH}\text{-}\underset{CHOH}{CH}\text{-}\overset{t}{CH{=}CH}\text{-}CH(OH)\text{-}(CH_2)_4\text{-}CH_3}\quad(\text{HOCH and CHOH joined by }\mathrm{CH_2})$$

(I)

PGF_{2-1} is thus a trihydroxy acid with two hydroxyl groups attached directly to a five membered hydrocarbon ring and the third along a carbon side chain

Table 6. *Final structure factors for the bromo derivative*

An asterisk marks changes in h and k. Each non-asterisk line contains l, $100A_o$, $100B_o$, $100A_c$ and $100B_c$

```
PLANES

*  0  1
3      0  -3288      0  -3133
*  0  2
2   6852      0   6749      0
*  0  3
2      0  -4530      0  -4365
3      0  -1692      0   -751
*  0  4
0  -2333      0  -3180      0
1  27261      0  30224      0
2   3220      0   4235      0
3  -1591      0  -1591      0
*  0  5
1      0   9864      0   9585
3      0   2467      0   2276
*  0  6
0   1047      0   2598      0
1  -4901      0  -4380      0
2   3836      0   3534      0
3   1495      0   1256      0
*  0  7
1      0  13983      0  13682
3      0   1848      0   2018
*  0  8
0  -5379      0  -5655      0
1  -7826      0  -7928      0
2   1345      0   1062      0
3   2596      0   1771      0
*  0  9
1      0   4039      0   3618
2      0   1158      0   1506
3      0   2700      0   2543
*  0 10
0   4374      0   4564      0
1  -5981      0  -5267      0
2  -2066      0  -2634      0
3   1686      0    200      0
*  0 11
1      0   6154      0   5544
2      0   1535      0   1350
3      0  -1936      0  -1507
*  0 12
0  -4033      0  -3954      0
1   4022      0   4807      0
*  0 13
1      0   7323      0   6730
2      0  -5151      0  -4929
3      0   2875      0   2725
*  0 14
1   3966      0   4199      0
2  -5824      0  -5743      0
3   2515      0   2356      0
*  0 15
1      0  -2435      0  -2354
2      0   2291      0   2087
3      0  -1523      0  -1121
*  0 16
0 -14770      0 -12133      0
1  -9787      0 -10050      0
2   4319      0   4821      0
*  0 17
1      0   3460      0   3200
2      0  -3540      0  -3105
3      0  -2795      0  -2754
*  0 18
0 -16018      0 -13602      0
1   5421      0   5692      0
*  0 19
1      0  -5690      0  -5861
3      0   1597      0   1103
*  0 20
0  12691      0  10935      0
1  -1504      0  -1702      0
2  -3208      0  -3367      0
*  0 21
2      0   2556      0   2525
*  0 22
0  -2807      0  -2295      0
1  -4456      0  -4157      0
*  0 23
1      0   1365      0   1745
2      0  -2167      0  -2145
*  0 24
0  -4371      0  -4206      0
1   4731      0   4397      0
*  0 25
1      0  -1240      0   -876
*  0 26
2  -1628      0  -2525      0
3  -1602      0  -1430      0
*  0 27
2      0  -2125      0  -3218
3      0  -2129      0  -1796
*  0 28
1   2148      0   1943      0
*  0 30
0   1945      0   2129      0
*  0 31
2      0   1416      0   1493
*  0 32
2    928      0   1120      0
*  0 34
0   1451      0   1459      0
*  0 36
1  -2132      0  -2140      0
*  0 37
1      0    967      0    793
*  0 38
1    919      0    400      0
*  1  0
2   1638      0   1240      0
3      0  -2948      0  -3345
*  1  1
2    349   -312    829   -741
3   1548   1154   1522   1135
*  1  2
2   7720  -2529   8396  -2751
3   2124  -1054   1462   -725
*  1  3
0      0  -1844      0  -1426
1   4944  10915   5905  13032
2  -2498   7288  -2561   7471
3   1605   1098   1129    773
*  1  4
0      0  -2391      0  -1606
1  -2351  -9630  -2232  -9145
2   -908   3025  -1190   3962
3  -3694    778  -2557    558
*  1  5
0      0   4528      0   4131
1   7220   7230   6992   7002
2   3837   2542   3763   2493
*  1  6
0      0   9852      0   8460
1 -15442   -104 -15609   -105
2  -3419   5805  -3420   5805
*  1  7
0      0  -5597      0  -3737
1   6895  -8704   6628  -8368
2   1536   2106   1432   1964
3  -1691   1346  -1274   1014
*  1  8
0      0  23347      0  20710
1  -9761   6639  -9071   6170
2   2692  -1734   2624  -1690
3  -1267  -1343  -1403  -1487
*  1  9
0      0   1016      0    421
1  -4358   -883  -4716   -956
2  -1412   -153  -1538   -167
3   1258   1612   1276   1636
*  1 10
0      0   5895      0   5679
1  -4017  -6966  -4051  -7024
2  -2505    736  -3149    926
3  -1574    616  -1697    665
*  1 11
0      0  -5767      0  -5354
1  -5422  -4858  -4735  -4242
2   3837  -2575   4361  -2940
*  1 12
0      0  -6959      0  -6241
1   -909   5589   -941   5791
2   1837   3343   2050   3736
*  1 13
0      0  -6880      0  -6206
1  -4298  10911  -4012  10186
2  -3618  -2240  -3367  -2084
3    -11  -1758    -10  -1733
*  1 14
0      0   2700      0   2767
1   -297  -2706   -205  -1868
2  -2317   -633  -2371   -646
3  -1952   2645  -1489   2018
*  1 15
0      0   7354      0   6886
1  -5633  -1341  -5326  -1268
2   -366  -2397   -309  -2021
3   1726   -533    697   -215
*  1 16
0      0   2288      0   2275
1  -5353  -2694  -5137  -2546
2    572   1321    521   1263
3   1430   1727   1367   1651

*  1 17
0      0  -7412      0 -12418
1   -400  -3584   -413  -3776
2   1042   3136   1079   3301
*  1 18
0      0   1744      0   1542
1   3180  -4577   2738  -2220
2   2930  -1273   2627  -1141
*  1 19
0      0  -2455      0  -2479
1  -1109   4189  -1306   4931
2  -1075  -2023  -1130  -2126
*  1 20
1   2012   1850   1910   1757
2  -1355    705  -3441   1019
*  1 21
0      0   6170      0   6035
1  -3968  -4529  -4156  -4745
2    278  -2073    266  -1786
*  1 22
1  -2775   1814  -2673   1747
2   1377  -1835   1401  -1875
*  1 23
0      0  -5173      0  -5061
*  1 24
0      0  -1918      0  -2199
1   3623  -2363   4041  -2636
2   -122  -1010    -82   -741
*  1 25
0      0   5132      0   4692
1   1078   2937   1217   3317
*  1 26
0      0  -5908      0  -5508
1    218   1449    338   2251
2  -1301    571  -1732    823
*  1 27
0      0   2071      0   1990
*  1 28
1   1546   2971   1672   3215
*  1 29
0      0   1454      0   1589
1  -2241     62  -2369     66
*  1 30
0      0  -2342      0  -2454
2  -1464   -338  -1827   -447
*  1 31
0      0  -1281      0  -1361
1   1726   -803   1668   -776
*  1 32
1    471   -992    743  -1567
2    894    526    795    468
*  1 34
1   1384    221   1582    273
*  1 35
0      0   2196      0   2476
*  1 37
1    693   -673    886   -860
*  1 39
1     25    863     46   1601
*  2  0
2    675      0    323      0
*  2  1
1 -12699   -159 -13096   -164
2   -193  -7386   -191  -7319
3    418   3962    297   2821
*  2  2
1   1271  11699   1319  12144
2  -4340  -2557  -4991  -2541
3   1648   1571   1222   1165
*  2  3
0  -4631      0  -5145      0
1   5474   4498   5346   4393
2  -1956   5768  -1858   5499
3  -1024  -1674  -1012  -1674
*  2  4
0  -5410      0  -4001      0
1  -8930   5305  -9246   5493
2  -2713  -2929  -2491  -2690
*  2  5
1  11396  -6800  12535  -7480
2  -8633  -2291  -8819  -2341
3   1219  -1965    627  -1010
*  2  6
0   3561      0   2760      0
1   1553  -1673   1341  -1445
2   1703   5125   1701   5118
*  2  7
0 -11668      0 -10465      0
1 -11197  -8287 -10575  -7827
2  -2118   2957  -2128   2472
3    752   2230    409   1214
*  2  8
0   8252      0   7795      0
1   4378   7347   3867   6491
2  -1613   1885  -1519   1776
*  2  9
0 -25705      0 -24245      0
1   3452   -266   2265   -132
2   2567  -1720   3041  -1632
*  2 10
0  -1996      0  -1832      0
1  -1175    574   -816    379
2   1327  -1782    950  -1286
3   -135   2430    -88   1585
*  2 11
0   4456      0   4542      0
1   2712  -1742   3214  -2065
2  -5451  -3280  -6121  -3083
3   -665   1611   -356    803
*  2 12
0   4683      0   4403      0
1   3791  -7293   3378  -6497
2   3765   2547   3318   2474
3   1761    133   1437    109
*  2 13
0  -6308      0  -6280      0
1  -9942   8371  -9681   8320
2  -5383   2289  -5831   2480
*  2 14
0   1715      0   1756      0
1  -5309  -5889  -5395  -5984
2   2622   -172   3314   -218
*  2 15
0  -7047      0  -7281      0
1   2460   3298   2287   3142
2   2751  -5975   2703  -4194
*  2 16
0  -4885      0  -4272      0
1   1815  -3003   2050  -3392
*  2 17
1   4633  -3509   4559  -3242
2    558   1272    598   1362
3  -1025   1842   -780   1408
*  2 18
0   4870      0   4443      0
1    -34  -4128    -37  -4552
2  -1213   -104   -510    -44
3   1428  -1203   1112   -984
*  2 19
0   1757      0   1605      0
1  -1211   2234  -1343   2476
2    465    458    702    463
*  2 20
0  -4156      0  -4185      0
1   -826  -1932   -984  -2300
2    542   1803    486   1620
*  2 21
0   2256      0   2831      0
1  -5366  -2513  -5361  -2509
2    332  -1489    236  -1060
*  2 22
0   4667      0   3140      0
1   2888   1167   3080   1244
*  2 23
0  -5190      0  -5524      0
1    299   1898    262   1663
2    988   1788   1172   2120
*  2 24
1  -2929  -2577  -3660  -5220
2   -554  -1612   -621  -1807
*  2 25
0   5873      0   4611      0
1   3267    413   3987    520
2  -1261   -589   -859   -402
*  2 26
0  -2987      0  -3103      0
1   1732  -2481   1999  -2865
*  2 27
1  -2802  -2529  -3083  -2775
*  2 28
0  10512      0   9953      0
1   2534   -367   3023   -438
*  2 29
0  -2907      0  -2211      0
1   2466   1332   3452   1551
2   1068     74    844     58
*  2 31
0   1882      0   3736      0
*  2 32
1   1255   1195   1403   1338
2   -681    707   -842   1121
*  2 36
1    186   -679    240  -1240

*  3  0
1      0  15067      0  15017
2   3170      0   3658      0
*  3  1
0      0   3182      0   3045
1  -8835   5111  -9317   5390
2  -1672   -231  -1911   -264
3  -2929   1322  -3276   1478
*  3  2
0      0  -1051      0   -551
1  -3689   7389  -3646   7302
2    -36  -1632    -25  -1121
3   2949    967   2755    641
*  3  3
0      0   2690      0   3743
1   1335    718    707    380
2   1185   3097   1299   3397
3   1409  -1579   1004  -1125
*  3  4
0      0  -7893      0  -7496
1   1585   6937   1426   6240
2     80  -1229     83  -1279
3    441  -1680    373  -1421
*  3  5
0      0   3525      0   2871
1  -1565   1507  -1563   1506
2  -1596   3446  -1642   3559
3  -2962   -637  -1830   -394
*  3  6
0      0  -2879      0  -2311
1   -981   -974  -1146  -1138
2   -465  -5330   -459  -5367
3  -1749    175  -1781    159
*  3  7
0      0  15463      0  13567
1 -11738   4744 -11468   4643
2   -496   -384   -652   -506
3    979   1486    815   1236
*  3  8
1  -5603  -7135  -5240  -6673
2  -2726   -527  -2757   -533
*  3  9
1   2576  -8217   2668  -8508
2   3473   -449   2845   -368
*  3 10
0      0  -7268      0  -7502
1  -2736   6871  -2803   7028
2   4117   -387   4265   -402
*  3 11
0      0  -9937      0  -9539
1   4377   6186   4267   6030
2  -6454   2457  -6165   2347
*  3 12
0      0   7645      0   7310
1   -192  -4065   -182  -3804
2   1157  -6998   1301  -7869
3  -1610   -984   -649   -397
*  3 13
1  -4570   5372  -4070   4784
2   -108  -3771    -87  -3032
3   2250  -2157   1954  -1010
*  3 14
0      0 -13030      0 -12530
1   1696  -6073   1626  -5821
2   -872  -3501   -767  -3160
3   1182   1536    763    991
*  3 15
0      0   2431      0   2937
1   3515  -1433   3298  -1345
2   3517    655   5488    649
3   -781   2052   -747   1962
*  3 16
0      0    791      0    557
1  -6005   5026  -5743   4807
2  -2225   -703  -2306   -763
*  3 17
0      0  -5402      0  -5297
1    233  -1437    151   -945
2  -2309    249  -1741    188
*  3 18
0      0   2273      0   1602
2   -830   -465   -730   -530
*  3 19
0      0  -4251      0  -3798
1   1742  -1576   1849  -1673
2    240  -2420    220  -2213
*  3 20
0      0   1388      0   1023
1   1439   -246   1068   -185
*  3 21
1   1894   2084   1652   2049
2  -1395  -1573  -1187  -1335
*  3 22
1   2354  -2598   2179  -2447
*  3 23
0      0   2012      0   2352
1   -505  -2507   -549  -2821
*  3 24
0      0  -1854      0  -1633
1  -1057   1360   -792   1019
*  3 25
0      0  -7375      0  -6641
1    639   1567    629   1343
2   -195   1301   -166   1109
*  3 26
0      0   7757      0   6660
1   3323    394   3979    472
*  3 27
0      0  40049      0   9656
1  -2698     14  -2823     15
2  -1555   -728  -1603   -750
*  3 28
1  -2194  -2483  -2634  -3108
2   -397   1460   -435   1598
*  3 29
0      0  -3927      0  -3843
1  -2810  -1831  -3053  -2015
2   -505   -747    347   -188
*  3 30
0      0  -5181      0  -4393
1    106   3150    100   2979
*  3 31
1   1168   1689   1101   1593
2   -803    490   -966    528
*  3 32
0      0   3979      0   3737
*  4  0
0  -4051      0  -4027      0
2   1899      0   1873      0
*  4  1
0   1581      0    676      0
1   6198   7669   6267   7755
2  -3344  -1260  -4032  -1552
*  4  2
0 -11765      0 -11930      0
1   8415 -14944   8265 -14678
2  -6001  -1602  -5779  -1343
*  4  3
0  15201      0  14210      0
1  -3546 -11102  -3473 -10872
2  -2126    474  -2001    459
*  4  4
0  13427      0  13026      0
1  -6145   5218  -6013   5175
2  -5297   1865  -5256   1871
*  4  5
0  -8437      0  -7596      0
1  -1327  -4620  -1243  -4327
2    750   1042    593    651
*  4  6
0 -13856      0 -14115      0
1  -6554  -1796  -6893  -1889
2   -685  -4261   -690  -4550
*  4  7
0   4791      0   3558      0
1   3439  -3548   3585  -3643
2   2603  -1341   2780  -1431
*  4  8
0 -13118      0 -12588      0
1   7887  -7599   7636  -7357
2    951   5266   1003   3050
*  4  9
0  15805      0  15716      0
1  -1508  -5816  -1582  -6203
2   -510    436   -733    927
*  4 10
0  14447      0  14235      0
1    144   5956    140   6040
2  -4096    991  -4098    991
*  4 11
0 -15180      0 -12374      0
1  -3019  -3201  -2795  -2964
2   1107    381   1476    355
3   -164  -2245   -149  -2034
*  4 12
0  -5690      0  -5325      0
1  -8469   -596  -8922   -628
2   4868  -1039   5122  -1093
3   2274   1770   2583   2011
*  4 13
0   -771      0   -200      0
1   6403  -5015   6860  -5328
2  -4437  -2851  -4056  -2991

*  4 14
0  -1038      0   -719      0
1   1732    566 [illegible]  565
2   4975   2977   2449   1724
*  4 15
0   2349      0   2269      0
1  -6370  -7353  -6412  -7412
2    132  -1963    166  -1603
*  4 16
0  10807      0  11346      0
1   -854   1405   -781   1270
2   2364  -4080   2587  -4454
*  4 17
0  -6062      0  -6240      0
1   2452   1026   2645   1166
2   2651  -2440   2685  -2472
*  4 18
0   3517      0   2702      0
1   -852  -2602   -244  -2514
2    354   2415    419   3090
*  4 19
0   4851      0   3879      0
1   1405   1286   1471   1328
*  4 20
1  -1020   3591  -1068   3758
2   2372    578   2981    508
*  4 21
0  -1043      0   -857      0
1  -2465   1501  -2827   1723
*  4 22
0   1244      0   1233      0
1   1997   -192   2095   -202
2   1732  -2469   1574  -2272
*  4 23
1   1125   -358    648   -229
*  4 24
0   4288      0   3517      0
1    580    819    890   1257
2  -1284   1465  -1354   1337
*  4 25
1  -2191    986  -2651   1193
2   -506   1842   -395   2375
*  4 26
1   -974    394   -445    180
2    -48  -1250    -34   -884
*  4 27
2    559  -1132    551  -1117
*  4 28
0   4219      0   4044      0
1   2659    735   2964    815
2    962   1656   1191   2048
*  4 29
0   3900      0   3640      0
1  -1141   2293  -1034   2079
*  4 30
1   1080   1747   1046   1692
2  -1133   -267  -1434   -338
*  4 32
2   -734   -554  -1085   -819
*  4 33
1   2011     90   1950     87
*  4 35
1  -1601   -242  -1814   -439
*  5  0
1      0 -23744      0 -25744
2  -1235      0  -1514      0
*  5  1
0      0  -6397      0  -6555
1 -15026   7145 -15585   6953
2   8920  -1573   9329  -1645
*  5  2
0      0 -25834      0 -23436
1    -77  22219    -71  20629
2  -2997    334  -3519    392
*  5  3
0      0   7227      0   5780
1   4775   5019   4947   5201
2  -2359  -4582  -2123  -4123
*  5  4
0      0  34102      0  28564
1   2707   -124   2658   -171
2  -2018  -4208  -2353  -4489
*  5  5
0      0  -1661      0  -1774
1  -9295  -5092  -7623  -5273
2  -2130  -2625  -1835  -2262
*  5  6
0      0 -19080      0 -16596
1   5930   -430   5648   -405
2   1684    327   2165    420
*  5  7
0      0 -10942      0 -10248
2   1229   1452   1476   1742
*  5  8
0      0  -6246      0  -5894
1   5401   2391   5151   2280
2   1067  -3511   1670  -3513
*  5  9
0      0  -2212      0  -2431
1   4726   3608   4809   3519
2  -1989  -2822  -1890  -2672
*  5 10
0      0  -5249      0  -5887
1   1202  -5035   1034  -4349
2  -1731   1155  -1822   1215
*  5 11
0      0   3516      0   4048
1  -3273  -3728  -3273  -3718
2    920   -547    845   -502
*  5 12
0      0  -2817      0  -3280
1   6473   6215   5654   5429
2   1656  -2433   1845  -2711
*  5 13
0      0   2265      0   1712
1   5235  -2613   5453  -2764
2  -5558   3552  -4001   3971
*  5 14
0      0  14102      0  12690
1   7096  -7250   6921  -6973
2   1537   -698   1094   -491
*  5 15
0      0   2909      0   1980
1  -3563   3240  -3213   2922
2  -1440    552  -1030    594
*  5 16
0      0  -6666      0  -7472
1  -1426   -354  -1257   -469
2  -1498   1880  -1558   2429
*  5 17
0      0   6916      0   6447
1   1028  -1067    878   -911
2   1921  -1244   2186   -931
*  5 18
0      0   1876      0   1638
1  -2365   4243  -2118   3799
2    408  -2429    283  -1683
*  5 19
0      0   1947      0   2507
1   2446  -4390   2176  -3906
2  -2388   2177  -2666   2430
*  5 20
0      0   2561      0   1711
1    181  -5479    108  -5085
2    976   -337    872   -301
*  5 21
1    448   2245    477   1653
2   1052   1979   1091   2052
*  5 22
0      0  -2729      0  -2359
1   -424   1212   -346   1045
2    -52   1401    -59   1586
*  5 23
0      0   2919      0   2346
1   2411   1256   2664   1389
*  5 24
0      0   3525      0   4313
1   -772    965   -633    792
*  5 25
0      0   2326      0   2023
1   -323  -2532   -348  -2733
*  5 26
0      0  -3148      0  -3293
1  -1179    520  -1452    646
*  5 27
1    448  -1637    452  -1051
2   1148    713   1492    927
*  5 28
1   -764   2511   -959   3152
2    941   -177   1805   -335
*  5 29
0      0  -2640      0  -2083
1   -548   1224   -544   1216
2  -1305    132  -1433    140
*  5 30
0      0  -2515      0  -2525
1   -819   -738   -795   -697
*  5 31
1   -821    908   -397    361
*  5 32
1   -474   1650   -601   2010
*  5 33
0      0  -1204      0  -1002
1    526   -609    936   -779
```

Table 6 (*cont.*)

•	5	34			
0		0	2869	0	2694
2		-85	-855	-41	-410
•	5	35			
1		-838	556	-1326	859
•	6	0			
0		20135	0	17755	0
1		0	-4375	0	-4118
•	6	1			
0		18164	0	16198	0
1		8114	-2128	7246	-1901
2		-4997	3194	-5056	3232
•	6	2			
0		19935	0	16315	0
1		-5968	-8200	-5771	-7930
2		197	763	168	631
•	6	3			
0		11889	0	9849	0
1		-14301	-880	-14776	-909
2		2626	-2102	2378	-1903
•	6	4			
0		-3487	0	-4143	0
1		3721	-6426	3661	-6321
2		-660	-3900	-637	-3761
•	6	5			
0		-1713	0	-1436	0
1		6014	-844	5510	-773
2		5650	1179	5724	1195
•	6	6			
0		9087	0	9453	0
1		1037	-3257	1197	-3762
2		-553	2786	-521	2623
•	6	7			
0		19174	0	17599	0
1		-1825	2655	-1841	2678
2		545	-678	500	-623
•	6	8			
1		-1492	-930	-1231	-767
2		3146	-2955	2795	-2625
•	6	9			
0		7705	0	7075	0
1		1359	-417	831	-255
2		2049	2333	1931	2200
•	6	10			
0		-725	0	-197	0
1		-2894	-2653	-2802	-2570
•	6	11			
0		15062	0	12466	0
1		426	5128	378	4552
2		1653	-3586	1445	-3130
•	6	12			
0		-6115	0	-5288	0
1		2046	5603	2343	6417
2		276	3117	302	3401
•	6	13			
0		-5989	0	-6141	0
1		750	-2143	867	-2478
2		2972	-473	3136	-501
•	6	14			
0		8512	0	7278	0
1		-3001	-1982	-2710	-1789
2		-757	-1756	-644	-1495
•	6	15			
0		16294	0	14123	0
1		3864	3623	5948	3675
2		762	1278	799	1339
•	6	16			
0		-4096	0	-3340	0
1		-3787	1453	-5991	1331
2		2399	1940	2652	1979
•	6	17			
0		4164	0	4748	0
1		-7672	441	-7577	433
2		950	-3127	952	-3133
•	6	18			
0		2326	0	1614	0
1		3560	6203	5410	5941
2		650	-939	768	-1109
•	6	19			
0		-12845	0	-11572	0
1		1818	466	2033	522
2		2205	206	2039	191
•	6	20			
1		-2242	-978	-1126	-887
2		-2492	-2148	-2410	-2078
•	6	21			
0		6336	0	3881	0
1		3619	945	4593	1196
2		-1584	969	-1345	943
•	6	22			
0		-5987	0	-5507	0
1		-985	1663	-1189	2009
2		769	2380	924	2859
•	6	23			
1		-3732	113	-3713	113
•	6	24			
1		3218	1589	2603	1286
•	6	25			
0		-5595	0	-4876	0
1		-362	1425	-299	1180
•	6	26			
1		-535	-1460	-411	-1790
2		-1182	642	-1040	565
•	6	27			
0		-2776	0	-2252	0
2		-308	-1318	-347	-1485
•	6	29			
1		717	1373	928	1777
2		-1106	-374	-1093	-364
•	6	30			
0		-1653	0	-2072	0
1		874	-1024	873	-1022
•	6	31			
0		3158	0	2816	0
1		-523	966	-347	641
2		-521	-769	-576	-851
•	6	32			
1		1428	773	1541	834
2		-1006	138	-1042	143
•	6	33			
0		-2180	0	-2007	0
1		-608	-1575	-708	-1834
•	6	34			
0		1235	0	1373	0
•	6	35			
1		1734	236	1774	242
•	6	36			
0		-1899	0	-1137	0
•	7	0			
1		0	9986	0	9657
2		3425	0	3887	0
•	7	1			
0		0	-14685	0	-12753
1		10049	2927	9465	2757
2		-7800	-892	-6723	-769
•	7	2			
0		0	5928	0	4838
1		-312	-2872	-326	-3003
2		856	-4525	749	-3952
•	7	3			
0		0	-9025	0	-8426
1		-1336	6135	-1403	6444
2		2974	-3411	2663	-3054
•	7	4			
0		0	1850	0	1631
1		5036	-1859	4625	-1708
2		-34	6019	-35	5865
•	7	5			
0		0	10364	0	9698
1		4311	-873	4282	-867
2		3022	-4419	5014	-4407
•	7	6			
0		0	8482	0	8069
1		440	4173	406	3846
2		-2208	3506	-2426	3852
•	7	7			
0		0	-8747	0	-8034
1		2779	-2812	2792	-2825
2		-2801	3579	-2643	3376
•	7	8			
0		0	11184	0	10291
1		2943	-1900	3050	-1969
2		2232	-295	1874	-248
•	7	9			
1		1556	6283	1525	6156
2		3359	1087	3515	1144
•	7	10			
0		0	6384	0	5803
1		5898	815	5620	777
2		-1033	1114	-618	667
•	7	11			
0		0	6216	0	5247
1		-4454	-2841	-4203	-2680
2		-2864	1118	-2254	880
•	7	12			
0		0	-5105	0	-1647
1		1792	-2661	2671	-2546
2		-1098	2016	-884	1623
•	7	13			
1		-4439	-2828	-4337	-2763
2		2412	4281	1969	3495
•	7	14			
0		0	-2409	0	-2333
1		-1040	1974	-1060	2012
2		-18	1858	-18	1817
•	7	15			
0		0	6088	0	5834
1		-606	1291	-262	557
2		1278	1093	1254	1073
•	7	16			
0		0	7048	0	7582
1		-3802	-170	-3804	-170
2		1659	-1207	1706	-1242
•	7	17			
1		-5988	97	-6675	108
2		-1332	-86	-1160	-72
•	7	18			
0		0	-3519	0	-2809
1		1721	-4588	1786	-4762
2		911	920	1016	1033
•	7	19			
0		0	6007	0	6219
1		-1797	86	-1880	90
2		2313	591	2215	566
•	7	20			
0		0	-4141	0	-4077
1		-2144	3472	-2328	3769
2		-1000	558	-1036	579
•	7	21			
0		0	-3640	0	-3485
1		468	-3557	446	-3388
2		-1619	1303	-1481	1192
•	7	22			
0		0	7594	0	7528
1		-1743	291	-2123	355
2		1317	-1893	1283	-1845
•	7	23			
1		-3215	3675	-3582	4095
•	7	24			
0		0	-8918	0	-8030
1		-208	-2859	-222	-3049
•	7	25			
0		0	5705	0	5853
1		1818	-1923	1666	-1763
2		706	-1480	619	-1298
•	7	26			
0		0	-1702	0	-1694
1		997	4128	1041	4313
•	7	27			
1		-2375	-388	-2015	-329
2		-1394	390	-1699	729
•	7	28			
2		-863	-925	-757	-811
•	7	29			
1		-353	1298	-479	1760
2		716	-918	755	-968
•	7	30			
0		0	-2817	0	-2237
•	7	31			
1		1093	-64	1313	-77
•	7	32			
1		-964	492	-1328	678
•	7	33			
0		0	-1252	0	-1457
1		60	1061	65	1153
•	7	34			
0		0	-1415	0	-1006
•	7	36			
0		0	-1149	0	1634
•	8	0			
0		7720	0	7314	0
1		0	12879	0	12991
2		4889	0	4601	0
•	8	1			
0		-9303	0	-10102	0
1		-5391	1971	-3239	1913
2		56	-4901	50	-4362
•	8	2			
0		11162	0	11331	0
2		1136	-1745	751	-1154
•	8	3			
0		8546	0	7977	0
1		2864	4306	2721	4091
2		2100	190	1875	170
•	8	4			
0		4818	0	4505	0
1		-3256	737	-3039	693
2		3344	820	2691	660
•	8	5			
0		6370	0	6085	0
1		-3341	3897	-3405	3971
2		-4133	-82	-4006	-79
•	8	6			
0		9359	0	8605	0
1		6175	1634	6268	1658
2		1786	-1082	2028	-1229
•	8	7			
0		-10372	0	-10882	0
1		-2288	5003	-2255	4931
2		-1337	3284	-1172	2878
•	8	8			
0		9299	0	8273	0
1		-7985	-183	-7228	-165
2		-2131	296	-2244	311
•	8	9			
1		5493	7727	5708	8030
2		-1078	-2481	-997	-2296
•	8	10			
0		-7876	0	-11264	0
1		-918	311	-1345	435
2		3438	77	2824	63
•	8	11			
0		2876	0	2265	0
1		-1931	5570	-1831	5340
2		-1988	-4407	-1886	-4180
•	8	12			
0		4424	0	4087	0
1		8435	-1354	8135	-1286
•	8	13			
0		-9029	0	-7694	0
1		-1977	6464	-1974	6454
2		-1584	2147	-1517	2057
•	8	14			
0		-2150	0	-1327	0
1		-3833	-492	-4029	-517
2		-2843	-579	-3500	-713
•	8	15			
0		-6364	0	-5589	0
1		1134	4241	1227	4588
2		807	490	857	520
•	8	16			
0		-8654	0	-8812	0
2		28	-2720	23	-2231
•	8	17			
1		2114	177	1917	161
2		781	-234	736	-221
•	8	18			
0		-3590	0	-2815	0
•	8	19			
0		1525	0	1566	0
1		-974	-564	-1152	-667
2		-1356	36	-1111	29
•	8	20			
0		-4860	0	-4582	0
1		1482	-1167	1249	-983
2		-330	1193	-307	1114
•	8	21			
0		-6043	0	-6807	0
1		-2769	-2441	-2625	-2313
•	8	22			
0		3252	0	2881	0
1		-1588	-1556	-1733	-1700
2		-2009	-902	-2351	-1055
•	8	23			
0		2358	0	2529	0
1		3980	-112	4207	-119
2		-66	927	-47	663
•	8	24			
0		-2414	0	-2133	0
2		856	1589	907	1472
•	8	25			
1		-4127	-784	-4676	-888
2		-752	-1465	-334	-1039
•	8	26			
0		1431	0	1193	0
1		3896	-2178	4530	-2333
2		-30	-1171	-33	-2078
•	8	27			
0		-3339	0	-2477	0
1		2190	-2793	2480	-3163
2		1661	1170	1959	1381
•	8	28			
0		5749	0	6005	0
•	8	29			
1		865	1031	808	964
2		-233	1032	-219	967
•	8	30			
0		-1654	0	-1308	0
1		-1037	-366	-1911	-674
2		911	-201	1198	-264
•	8	31			
0		1805	0	2577	0
2		-160	-1108	-222	-1545
•	8	32			
1		1403	204	2140	311
•	8	33			
0		1605	0	550	0
•	8	36			
0		-1132	0	-18	0
•	9	0			
1		0	3716	0	4071
2		-927	0	-954	0
•	9	1			
0		0	13188	0	12618
1		1008	-2069	1138	-2337
2		-490	4146	-479	4051
•	9	2			
0		0	2180	0	1816
1		-1698	6124	-1688	6089
2		-2618	602	-2567	590
•	9	3			
0		0	7568	0	6716
1		5323	-1925	5215	-1886
2		-2542	5916	-2592	6032
•	9	4			
0		0	7541	0	6706
1		-7414	-1508	-7686	-1563
2		5644	1912	5462	1850
•	9	5			
1		1475	7115	1551	7484
2		1500	-94	1007	-63
•	9	6			
0		0	-3924	0	-3998
1		375	-1967	309	-1621
2		-1656	1555	-1755	1470
•	9	7			
0		0	12876	0	12609
1		852	1015	1205	1435
2		2398	-1575	2003	-1315
•	9	8			
0		0	5477	0	5860
1		-7334	1491	-7032	1698
2		-3318	356	-2942	316
•	9	9			
0		0	2672	0	2341
1		-2111	-8186	-1930	-7485
2		1698	3651	1850	3979
•	9	10			
0		0	11263	0	11203
1		-4145	-3244	-4463	-3492
2		6251	-1658	6291	-1663
•	9	11			
0		0	-12110	0	-11982
1		-5004	6137	-5001	7360
2		394	1540	351	1373
•	9	12			
0		0	-7415	0	-6421
1		4695	3327	4320	3061
2		-813	1114	-703	1047
•	9	13			
0		0	7488	0	6920
1		929	2633	1011	2807
2		-1929	-3748	-2164	-4214
•	9	14			
0		0	6310	0	6250
1		-5521	1257	-5728	1307
2		1279	-661	1024	-689
•	9	15			
0		0	-8614	0	-8536
1		-3198	-935	-3554	-1039
•	9	16			
0		0	-3474	0	-2935
•	9	17			
0		0	-5333	0	-4923
1		-2243	2639	-2374	2793
2		511	-1412	395	-1864
•	9	18			
1		-1413	-729	-1342	-673
2		-2097	-746	-2373	-844
•	9	19			
0		0	-3726	0	-3122
1		-729	-1487	-1199	-1918
2		-294	-1424	-240	-1244
•	9	20			
0		0	-2452	0	-2328
1		666	-2551	586	-2242
2		866	495	659	377
•	9	21			
0		0	-1950	0	-1756
2		1548	-1317	1225	-1043
•	9	22			
0		0	-2828	0	-2736
1		2118	2890	1907	2602
2		-1880	-2060	-1735	-1901
•	9	23			
0		0	1671	0	806
1		720	-2088	973	-2072
2		-1260	-412	-1059	-543
•	9	24			
2		2040	-918	2316	-1039
•	9	25			
0		0	-1230	0	-1196
1		-359	1893	-272	1436
2		-2066	-246	-2233	-260
•	9	26			
0		0	-1250	0	-684
1		1575	-1152	1584	-1159
2		399	1610	443	1780
•	9	27			
0		0	1634	0	1596
1		-1481	1046	-1174	829
2		85	-1510	70	-1236
•	9	28			
0		0	-1805	0	-1146
1		-909	552	-1014	616
•	9	29			
0		0	1181	0	211
1		323	-2434	403	-3041
•	9	30			
2		474	-1029	658	-1429
•	9	31			
0		0	-1642	0	-1863
1		-85	1525	-97	1754
2		71	1104	97	1509
•	9	33			
0		0	3087	0	3722
•	10	0			
1		0	1301	0	1229
2		-2738	0	-2554	0
•	10	1			
0		-5533	0	-5268	0
1		994	6659	1022	6841
2		-1385	-494	-633	-197
•	10	2			
0		-8443	0	-8739	0
1		-553	3118	-599	3378
2		947	697	1024	754
•	10	3			
0		-1661	0	-1696	0
2		-1074	-6095	-1113	-6319
•	10	4			
0		6038	0	5881	0
1		9431	5418	8796	5053
2		-3613	-2513	-4106	-2856
•	10	5			
0		4172	0	3925	0
1		63	-6418	67	-6770
2		-4974	4093	-5093	4806
•	10	6			
0		-2550	0	-2268	0
1		-7702	3466	-8431	3794
•	10	7			
0		-5883	0	-5594	0
2		-3346	-1074	-3155	-1013
•	10	8			
0		-11753	0	-11235	0
1		5704	859	5292	797
2		-871	2893	-878	2916
•	10	9			
0		-11512	0	-10738	0
1		3244	-5221	2969	-4779
2		-861	-47	-619	-34
•	10	10			
0		9207	0	9488	0
1		-4179	-3682	-3055	-2691
2		-398	1578	-1027	1805
•	10	11			
0		-7905	0	-6928	0
1		2186	1264	1955	1119
2		-3554	284	-3595	288
•	10	12			
0		-8299	0	-7736	0
1		-2726	-2627	-2558	-2405
2		2244	1628	2364	1710
•	10	13			
0		-3637	0	-3982	0
1		-3971	-6117	-4142	-6336
2		-3392	-3450	-3603	-3697
•	10	14			
0		2293	0	932	0
1		7125	-3498	7916	-3886
•	10	15			
0		-1925	0	-1641	0
1		-2374	-4393	-2391	-4423
2		-50	4127	-49	4045
•	10	16			
0		6305	0	5565	0
1		-1203	-3315	-1129	-3112
2		-1628	-1508	-1661	-1539
•	10	17			
0		2274	0	1574	0
1		3160	-1519	2693	-1294
2		140	-1031	209	-1348
•	10	18			
1		-2209	-1856	-2438	-2048
2		3454	-298	3369	-290
•	10	19			
0		1659	0	1476	0
1		1651	-568	1434	-500
2		12	-1257	12	-1270
•	10	20			
0		1293	0	849	0
1		1259	-2270	1212	-2185
2		2016	182	2143	193
•	10	21			
1		-1284	1174	-1689	1344
2		1866	-576	2535	-783
•	10	23			
0		-1199	0	-1061	0
1		-1947	-178	-2514	-230
2		2300	-683	2395	-712
•	10	24			
0		3802	0	2962	0
1		1763	-751	2163	-921
2		-928	-707	-1112	-847
•	10	25			
0		1243	0	2114	0
1		-1314	1327	-1463	1477
2		-694	1650	-793	1886
•	10	26			
0		1260	0	1286	0
1		-841	-697	-301	-415
•	10	27			
0		4334	0	5251	0
1		-570	1216	-691	1474
•	10	28			
0		-1478	0	-1231	0
1		2172	2927	2277	3068
•	10	29			
1		-373	-1034	-355	-978
•	10	30			
0		4037	0	3532	0
2		-924	-437	-906	-428
•	10	31			
0		-1460	0	-1520	0
1		2018	1845	2035	1861
2		741	665	807	724
•	10	32			
0		-3214	0	-2612	0
1		[illegible]	-894	-1968	-925
•	10	33			
0		2534	0	2453	0
•	10	34			
1		1289	227	1912	337
•	10	35			
1		-1229	-253	-1472	-302
•	11	0			
1		0	-2750	0	-3276
2		-1237	0	-472	0
•	11	1			
0		0	6243	0	6403
1		-5282	-4776	-9708	-4840
2		770	-2340	537	-2846
•	11	2			
0		0	-8242	0	-8405
1		-3114	-1656	-2855	-1519
2		1710	442	1410	365
•	11	3			
0		0	915	0	811
1		-2376	3712	-2520	3937
2		2530	3477	2458	3392
•	11	4			
0		0	2519	0	2520
1		-3990	6740	-4183	7065
2		755	-3969	693	-3641
•	11	5			
0		0	11356	0	10556
1		-5662	6912	-5815	7099
2		-1300	-514	-1533	-415
•	11	6			
1		-3235	-1230	-3461	-1292
2		-1070	-3527	-1143	-3733
•	11	7			
0		0	-12329	0	-10860
1		-3992	-353	-3290	-296
2		75	1874	79	1578
•	11	8			
0		0	-5897	0	-8050
1		2768	-11	2690	-17
2		1415	-1324	1807	-1680
•	11	9			
0		0	-2451	0	-903
1		-2165	4205	-2270	4409
2		1232	-512	95	-24
•	11	10			
0		0	-13831	0	-12946
1		-1856	2529	-2189	2984
2		-2216	-1692	-2185	-1669
•	11	11			
0		0	-2674	0	-2307
1		3459	-7330	3477	-7367
2		-951	-1070	-968	-1123
•	11	12			
0		0	936	0	859
1		-1630	1901	-1531	1787
2		1366	-3374	1324	-3269
•	11	13			
1		2558	2191	2713	2324
2		-3864	-441	-4520	-517
•	11	14			
1		1886	-5758	1957	-5973
•	11	15			
0		0	9783	0	8856
1		1569	-578	2043	-753
2		1195	-1978	849	-1406
•	11	16			
0		0	-3278	0	-3554
1		-3183	1740	-3006	1644
2		-2524	-55	-2143	-46
•	11	17			
0		0	-8273	0	-8259
1		2312	-1434	3037	-1896
2		-425	760	-446	799
•	11	18			
0		0	4829	0	4736
1		-134	2540	-134	2541
2		1670	-1276	1738	-1328
•	11	19			
0		0	-1707	0	-1724
1		308	3669	307	3653
2		-526	1475	-469	1316
•	11	20			
1		2199	-3054	2355	-3550
2		-825	892	-1209	1307
•	11	21			
0		0	3043	0	3609
1		2055	-3357	2457	-4014
•	11	22			
0		0	-2877	0	-2789
2		88	2106	97	2330
•	11	23			
0		0	1693	0	1429
1		1199	-2213	1157	-2135
2		-1043	-1083	-1490	-1548
•	11	24			
2		1520	-943	1310	-813
•	11	25			
0		0	3703	0	3579
1		1063	-800	1188	-894
•	11	26			
0		0	3529	0	3814
1		-1098	-35	-1248	-40
•	11	27			
0		0	-1476	0	-2111
1		-632	2096	-526	1657
2		166	934	286	1613
•	11	29			
1		-546	1640	-425	1276
•	11	30			
0		0	-1940	0	-2475
1		1128	1026	1540	1401
2		-1145	330	-833	240
•	11	31			
1		116	-1981	137	-2340
2		479	853	372	662
•	11	32			
0		0	1740	0	836
1		-1042	1030	-1074	1062
2		832	-139	695	-116
•	11	33			
0		0	-1832	0	-2190
2		-935	325	-765	266
•	11	34			
1		818	-1299	731	-1101
•	11	35			
0		0	1574	0	3212
1		-541	283	-438	717

Table 6 (*cont.*)

• 11	30			
0	0	-1370	0	-1526
• 12	0			
0	-11577	0	-11537	0
1	0	-1367	0	-446
2	-1305	0	-150	0
• 12	1			
0	2154	0	2153	0
1	4114	-4732	3710	-4207
2	-2548	2019	-2384	1890
• 12	2			
0	-2024	0	-1118	0
1	3783	-2644	3814	-2666
2	-3516	1777	-3290	1003
• 12	3			
0	837	0	965	0
1	-3763	-3701	-3817	-3754
2	1482	3261	1633	3594
• 12	4			
0	-4317	0	-2986	0
1	-6547	-2809	-6178	-2050
2	-3518	-565	-3603	-578
• 12	5			
0	2911	0	2540	0
1	1102	-6169	1013	-5707
2	430	-3185	351	-2602
• 12	6			
1	-2162	-4157	-2301	-4424
• 12	7			
0	10338	0	9731	0
1	-972	-3105	-1062	-3392
2	978	-12	832	-10
• 12	8			
0	5611	0	4655	0
1	-1950	-1394	-2102	-1503
2	-1051	160	-710	168
• 12	9			
0	3583	0	3004	0
2	686	-1122	1227	-1553
• 12	10			
1	2825	-1618	2477	-1419
2	2104	1266	2050	1234
• 12	11			
1	653	-4481	679	-4659
2	1069	-1416	836	-1107
• 12	12			
0	4886	0	4312	0
2	-329	934	-462	1311
• 12	13			
0	5891	0	5452	0
1	1791	223	2017	251
2	1728	2378	1477	2033
• 12	14			
0	-2850	0	-2613	0
1	-4283	-2060	-4290	-2070
2	3372	1500	3707	1649
• 12	15			
0	10000	0	9272	0
2	2251	-2859	2028	-2669
• 12	16			
0	2676	0	3022	0
1	1138	1561	1039	1426
2	1267	2033	1487	1213
• 12	17			
0	1785	0	1647	0
1	-4475	-884	-4329	-855
2	-468	-1080	-103	-237
• 12	18			
0	10069	0	9467	0
1	-1720	3939	-1522	3487
2	-1758	-3163	-1628	-2929
• 12	19			
0	-5048	0	-4630	0
1	4061	2009	4105	2030
2	1289	-166	1766	-227
• 12	20			
1	-2771	-452	-1481	-242
2	1220	-167	789	-108
• 12	21			
0	4226	0	3744	0
2	-405	-1353	-402	-1342
• 12	22			
1	5602	417	6384	476
2	1622	727	2038	914
• 12	23			
0	-3433	0	-3209	0
1	-2198	1811	-2188	1803
2	672	2084	604	1874
• 12	24			
2	-212	1050	-221	1094
• 12	25			
0	-2424	0	-2070	0
2	-446	-1083	-634	-1341
• 12	26			
0	-2210	0	-1605	0
1	-1762	-716	-2309	-938
2	773	-798	777	-638
• 12	28			
1	-795	1080	-826	1114
2	315	-872	192	-533
• 12	29			
1	326	1577	372	1521
2	-1040	-397	-1001	-382
• 12	31			
0	1566	0	1501	0
1	1180	652	1415	721
2	-878	-422	-619	-349
• 12	34			
1	-815	-676	-1191	-914
• 12	35			
0	1536	0	2768	0
• 12	36			
0	-1329	0	-1719	0
• 13	0			
1	0	6257	0	6164
• 13	1			
0	0	-12842	0	-12610
1	1731	1616	1627	1677
2	-2349	-1752	-2276	-1703
•	2			
0	0	-1626	0	-1381
1	7013	-2750	7690	-2778
2	-1776	-1945	-1687	-1661
• 13	3			
1	-2909	-1190	-2480	-1015
2	770	-3220	676	-2826
• 13	4			
0	0	-6176	0	-3484
1	-1308	1528	-1123	1398
2	590	2590	636	2433
• 13	5			
0	0	-5916	0	-5562
1	-1965	-2343	-2024	-2413
2	1319	-2869	1091	-2372
• 13	6			
0	0	7479	0	7830
1	4170	3157	4425	3350
2	2226	-2289	2082	-2141
• 13	7			
0	0	-2566	0	-2189
1	140	2558	160	2933
2	-2549	1716	-2357	1387
• 13	8			
0	0	-4054	0	-3831
1	4387	-2325	4812	-2550
2	-341	-1821	-454	-2429
• 13	9			
0	0	6275	0	5867
• 13	10			
0	0	-3878	0	-4347
1	2505	2562	2684	2744
• 13	11			
2	-1199	-498	-629	-261
• 13	12			
1	5214	-2436	5289	-2572
2	-1762	171	-1987	216
• 13	13			
0	0	3042	0	2780
1	-345	-2000	-452	-2622
2	2052	3272	2154	3433
• 13	14			
0	0	-3020	0	-3366
1	-18	-1309	-27	-1934
2	2962	105	2841	101
• 13	15			
1	1475	260	1005	177
2	2513	1788	2620	1865
• 13	16			
0	0	2704	0	2253
1	-874	-416	-354	-109
2	520	-1062	518	-1058
• 13	17			
0	0	3314	0	3696
1	-766	793	-867	897
2	-525	-1907	-307	-1114
• 13	18			
1	-465	893	-410	787
2	-407	1237	-252	766
• 13	19			
0	0	-3354	0	3510
1	-561	-2837	-515	-2605
2	757	855	460	520
• 13	20			
0	0	2756	0	2625
1	-1060	2418	-1099	2505
2	79	-1050	36	-470
• 13	21			
1	29	2110	44	2422
2	-1438	1878	-1556	2032
• 13	22			
1	337	-4902	294	-4274
2	-1143	1575	-1292	1782
• 13	23			
0	0	5172	0	6174
1	-901	-1236	-772	-1057
• 13	24			
0	0	-4360	0	-3935
2	943	1163	1122	1409
• 13	25			
1	796	-2188	690	-1898
2	1368	1142	1118	934
• 13	26			
0	0	3746	0	3464
1	-402	1285	-384	1227
• 13	27			
1	-1003	706	-957	673
• 13	30			
0	0	-1440	0	-1515
• 13	35			
0	0	-1429	0	-1815
• 13	36			
0	0	1404	0	628
• 14	0			
0	7510	0	6645	0
1	0	-1147	0	-1192
2	-1018	0	-423	0
• 14	1			
1	-1284	-82	-744	-48
2	427	-1140	213	-570
• 14	2			
0	1192	0	1046	0
1	-1680	-4614	-1809	-5182
2	1221	712	1927	1123
• 14	3			
0	6967	0	7016	0
1	-1902	1054	-1815	1006
• 14	4			
0	1619	0	1249	0
1	1769	-3048	1781	-3177
2	1618	1356	1861	1560
• 14	5			
0	4149	0	4246	0
1	-4227	1311	-4174	1295
2	1929	529	1796	493
• 14	6			
0	7422	0	8152	0
1	-2526	-1592	-2505	-1578
2	159	-4876	142	-4377
• 14	7			
0	1115	0	748	0
1	3730	3422	3344	3068
2	867	-1354	815	-1273
• 14	8			
0	-2039	0	-1350	0
1	-2406	-3630	-2438	-3678
2	1412	-993	791	-556
• 14	9			
0	10973	0	11887	0
1	351	1928	359	1972
2	-325	-956	-255	-751
• 14	10			
0	2106	0	2171	0
1	2703	4193	2632	4081
• 14	11			
0	-2302	0	-2254	0
1	-1932	3977	-2137	4422
2	1156	2088	1368	2288
• 14	12			
1	-1594	459	-1701	501
2	-1930	-1396	-1754	-1269
• 14	13			
0	-1511	0	-1529	0
1	3310	968	3530	1032
• 14	14			
0	1406	0	1869	0
1	-265	1892	-145	2036
2	1254	1088	1065	924
• 14	15			
0	-1282	0	-971	0
1	-1649	2555	-1473	2597
2	107	1186	101	1113
• 14	16			
0	-2264	0	-1680	0
1	-2283	1620	-3150	2249
2	-87	-2261	-78	-2016
• 14	17			
1	1202	2262	1108	2085
2	984	-2063	989	-2081
• 14	18			
0	-3654	0	-3368	0
1	1961	1892	2235	2156
2	67	1234	30	554
• 14	19			
1	-1777	-1123	-2426	-981
2	-340	-1290	-280	-1060
• 14	20			
0	2719	0	2725	0
1	582	1376	479	1278
2	-1200	-1613	-1583	-1965
• 14	21			
0	-4025	0	-3679	0
1	495	817	617	1019
• 14	22			
0	-2042	0	-2407	0
1	-233	-1306	-252	-1414
• 14	23			
1	861	2035	907	2145
2	-1391	596	-948	406
• 14	24			
0	-2207	0	-2091	0
1	1317	817	1496	927
2	147	1500	140	1423
• 14	25			
0	-1478	0	-1742	0
1	-2059	-1339	-2065	-1343
• 14	26			
0	1634	0	1801	0
2	-829	-1027	-674	-835
• 14	27			
0	-2445	0	-2667	0
1	1160	-1146	747	-738
2	1207	476	1500	592
• 14	28			
1	-1440	-489	-1466	-498
• 14	29			
0	1252	0	1776	0
2	-1132	-491	-1402	-603
• 14	30			
1	1362	151	1452	163
• 14	31			
1	-1400	-252	-1539	-277
• 14	33			
1	892	-852	1377	-1315
• 14	35			
0	1436	0	873	0
• 15	0			
1	0	-1476	0	-1936
2	-3616	0	-3199	0
• 15	1			
0	0	1705	0	1383
1	2358	-2122	1975	-1777
2	1755	947	1953	1057
• 15	2			
1	-358	1875	-395	2072
2	-735	1049	-473	685
• 15	3			
0	0	-2170	0	-2205
1	6303	-573	6939	-623
2	-1160	301	-1014	316
• 15	4			
0	0	6991	0	9246
1	928	-1995	993	-1625
2	1354	1565	1270	1490
• 15	5			
0	0	-1712	0	-849
1	193	2052	156	1656
2	999	-602	630	-561
• 15	6			
1	1124	1290	621	870
2	-63	2542	-59	2380
• 15	7			
0	0	4372	0	3886
1	2283	-284	2573	-321
2	2938	935	2618	828
• 15	8			
0	0	10113	0	9570
1	38	4253	30	4046
2	518	-1714	653	-2163
• 15	9			
0	0	1197	0	1586
1	-2078	543	-2355	615
2	-3537	1274	-3290	1185
15	10			
	0	4138	0	3550
	1503	-4207	1724	-4827
	73	2724	71	2639
• 15	11			
1	-1688	811	-1419	630
2	2869	-345	2801	-332
• 15	12			
1	2673	2078	2727	2174
2	-76	2581	-76	2575
• 15	13			
1	1141	-331	1189	-344
2	-1374	963	-1303	913
• 15	14			
0	0	5325	0	5275
1	373	1592	460	1962
2	1618	518	1466	467
• 15	15			
1	-3471	761	-3310	725
2	-977	1557	-1065	1694
• 15	16			
1	-1140	-2318	-1034	-2103
• 15	17			
1	-581	858	-620	916
2	1304	-246	1571	-297
• 15	18			
1	186	1035	283	1572
2	402	1276	402	1278
• 15	19			
0	0	1865	0	1519
1	-2940	505	-2585	442
2	-731	-1026	-821	-1152
• 15	20			
1	-1672	-108	-1361	-137
• 15	21			
0	0	1446	0	2009
1	-986	-1041	-1012	-1009
2	790	1101	655	912
• 15	22			
0	0	-2066	0	-2020
1	-2627	511	-2751	574
• 15	23			
0	0	-2327	0	-2650
2	-1560	439	-1586	523
• 15	24			
2	894	-735	1065	-875
• 15	25			
1	-1585	1038	-1193	781
2	-176	-1029	-94	-549
• 15	26			
0	0	-3623	0	-2908
2	-585	708	-245	296
• 15	27			
1	259	-1688	196	-1277
2	998	-1108	1249	-1387
• 15	28			
1	-1081	2114	-1077	2105
2	89	-1135	133	-1727
• 15	29			
0	0	-3423	0	-2643
2	-848	-6	-1342	-9
• 15	30			
1	968	-1778	1112	-2042
• 15	31			
0	0	1354	0	1584
1	-643	1718	-541	1447
• 15	32			
0	0	-2067	0	-2582
• 15	34			
1	-405	1151	-350	979
• 16	0			
0	6112	0	6415	0
1	0	1781	0	1562
2	1025	0	909	0
• 16	1			
0	1435	0	827	0
1	582	1564	726	1949
2	-1771	-849	-1092	-523
• 16	2			
0	5378	0	4570	0
1	-489	1939	-601	2381
2	2186	826	2072	783
• 16	3			
0	-1353	0	-2395	0
1	-1154	3546	-1211	3722
2	525	-982	674	-1260
• 16	4			
1	1269	2579	1051	2201
2	2218	-1160	2156	-1128
• 16	5			
1	3241	543	2871	481
2	124	-1341	90	-1063
• 16	6			
0	2823	0	3319	0
• 16	7			
1	-3723	1788	-4099	1968
2	-3080	-353	-3288	-590
• 16	9			
0	-6263	0	-6367	0
1	995	3382	1033	3510
2	-790	1446	-724	1327
• 16	10			
1	-1784	-188	-1492	-157
• 16	11			
0	2875	0	2678	0
1	1196	3236	1219	3298
2	-1853	-2079	-1979	-2221
• 16	12			
0	-4800	0	-4346	0
1	2778	1050	3320	1262
2	-1005	477	-1141	542
• 16	13			
0	-4873	0	-4305	0
1	-1846	-1542	-2123	-1774
2	-1432	947	-1226	811
• 16	14			
1	1814	-1449	2097	-1675
2	-1722	-684	-1077	-666
• 16	15			
0	-3061	0	-2908	0
1	2879	-645	2461	-552
2	731	592	796	656
• 16	16			
0	-3106	0	-3099	0
1	-1057	-1635	-979	-1346
2	-1253	-66	-1263	-65
• 16	18			
0	-4181	0	-4519	0
• 16	19			
0	-4052	0	-3787	0
2	-957	194	-1384	287
• 16	20			
1	116	-2767	132	-3142
• 16	21			
1	-1135	-282	-1261	-979
2	65	-1551	54	-1166
• 16	22			
1	872	-1017	1027	-1198
• 16	23			
2	1515	616	1640	667
• 16	25			
1	1045	-321	700	-215
• 16	26			
1	353	-1023	318	-923
• 16	27			
1	-1967	-51	-2035	-52
• 16	28			
1	905	901	722	789
• 16	29			
0	-1561	0	-1292	0
	846	-972	602	-406
• 16	30			
1	-1191	-1107	-1167	-1173
• 16	31			
0	1526	0	2398	0
• 16	33			
1	-1154	-117	-1543	-139
• 16	34			
0	2207	0	2223	0
• 16	35			
1	480	688	774	1110
• 17	0			
1	0	1612	0	1087
• 17	1			
0	0	6144	0	3715
1	-84	-407	-292	-1405
2	-832	247	-717	213
• 17	2			
0	0	2033	0	2225
1	-2273	-2120	-2498	-2330
2	831	258	1335	414
• 17	3			
0	0	3888	0	3574
1	302	1847	269	1644
2	602	2086	370	2630
• 17	4			
0	0	-1142	0	-1565
1	-2781	479	-2634	434
• 17	5			
0	0	2641	0	2803
1	2025	1372	1368	1289
2	887	1779	704	1411
• 17	6			
0	0	4982	0	3449
1	-2614	537	-2358	322
2	437	-1174	418	-1123
• 17	7			
0	0	2282	0	2274
1	-2749	1144	-2474	1222
2	-262	962	-429	1221
• 17	8			
1	-3186	-1315	-3441	-1678
2	1456	1768	1559	1522
• 17	9			
1	-1969	24	-2136	38
2	2174	150	2179	149
• 17	10			
1	-3772	3467	-4273	3916
2	220	-1272	244	-1429
• 17	11			
0	0	-3364	0	-3980
2	-1346	-853	-1723	-1111
• 17	12			
0	0	2522	0	1806
1	-2086	-3037	-1927	-1582
2	-827	-779	-647	-609
• 17	13			
1	-2172	-190	-2407	-210
• 17	14			
0	0	-4678	0	-4149
1	-3060	1174	-3407	1307
2	227	1028	149	674
• 17	15			
2	3	-1895	3	-2037
• 17	16			
1	-2645	1787	-2605	1760
2	-689	-1055	-672	-1039
• 17	17			
0	0	-7319	0	-7499
2	-1084	-938	-836	-723
• 17	18			
1	1447	-1938	1521	-2036
• 17	19			
1	-339	2246	-387	2565
2	912	-1385	747	-1134
• 17	20			
0	0	-3569	0	-3284
1	147	1089	101	749
• 17	21			
0	0	2446	0	2746
1	185	-1333	191	-1375
• 17	23			
0	0	-1812	0	-1658
• 17	24			
0	0	-1649	0	-1516
• 17	25			
1	1305	196	1404	211
• 17	28			
1	1325	-347	1805	-449
• 17	29			
1	-94	-1102	-49	-569
• 17	30			
1	250	923	249	917
• 17	32			
0	0	1607	0	2041
• 17	33			
1	-809	1300	-1045	1679
• 18	0			
0	-6975	0	-7281	0
1	0	3225	0	3686
• 18	1			
0	-2550	0	-3273	0
1	-317	-919	-371	-1078
• 18	2			
1	1843	1952	1949	2064
2	-1959	-687	-2128	-754
• 18	3			
0	-2511	0	-2511	0
1	1945	-45	2280	-52
2	-2013	804	-1983	792
• 18	4			
0	-3642	0	-3292	0
1	-2832	2005	-3055	2163
2	-1901	678	-2082	743
• 18	5			
1	497	-852	785	-1347
2	-1161	-955	-840	-691
• 18	6			
0	-3058	0	-3716	0
1	833	1631	840	1661
• 18	7			
0	-3716	0	-4326	0
1	-647	-2132	-695	-2289
2	-2286	-425	-2240	-416
• 18	8			
1	-213	-3358	-249	-4161
2	-781	2146	-726	1995
• 18	9			
1	-1103	-2846	-980	-2528
• 18	11			
0	-3740	0	-3172	0
1	483	-1943	544	-2183
2	-1736	252	-1921	279
• 18	12			
0	1952	0	1638	0
1	-242	-3237	-257	-3463
2	-420	844	-567	1141
• 18	13			
0	1709	0	1651	0
2	-608	1286	-565	1191
• 18	14			
1	-1147	-2079	-1308	-2371
2	965	1157	1165	1400
• 18	15			
0	3703	0	3613	0
1	-1666	320	-1263	242
2	379	-999	368	-970
• 18	16			
0	1439	0	1714	0
1	1293	-606	1637	-767
• 18	17			
1	504	-2113	590	-2474
2	1689	599	1709	606
• 18	18			
0	2533	0	2900	0
1	-1523	-253	-1624	-270
2	620	729	625	735
• 18	19			
0	1374	0	1801	0
2	-896	325	-1169	424
• 18	20			
1	980	-1204	1155	-1420
2	1338	-45	1618	-52
• 18	21			
1	-2052	-61	-2017	-60
2	1617	-475	1701	-521
• 18	22			
0	5306	0	5346	0
1	697	-1007	1038	-1498
• 18	23			
1	291	1050	293	1059
• 18	33			
1	623	707	786	892
• 18	34			
0	-1339	0	-772	0
• 19	0			
2	2337	0	1627	0
• 19	1			
1	-3003	1727	-2752	1582
2	1326	63	1139	59
• 19	2			
0	0	-3318	0	-3432
2	-404	-1054	-194	-505
• 19	3			
0	0	1153	0	1342
1	-3546	-475	-3434	-460
2	-679	-1013	-413	-618
• 19	4			
0	0	-2834	0	-2776
1	-1328	897	-1419	958
2	325	-2232	353	-2475
• 19	5			
0	0	-4050	0	-3895
1	-2919	-25	-2727	-24
2	-374	1564	-397	1661
• 19	6			
0	0	-3508	0	-3463
1	971	-1069	965	-1062
2	845	-1636	807	-1610
• 19	7			
0	0	3039	0	2894
1	384	2971	354	2738
• 19	8			
0	0	-1936	0	-1751
1	-93	1933	-95	1985
2	-932	-946	-503	-511
• 19	9			
2	-1741	-1190	-1820	-1244
• 19	10			
0	0	-3352	0	-3502
2	371	-2635	421	-2994
• 19	11			
0	0	-2106	0	-2077
1	655	1345	656	1344
2	584	-1113	514	-980
• 19	12			
0	0	-4709	0	-4785
2	-82	-1579	-72	-1383
• 19	13			
2	955	36	1470	38

Table 6 (*cont.*)

• 19	14			
0	0	-1440	0	-1219
2	821	-837	509	-519
• 19	15			
0	0	-1022	0	-1634
1	1253	1180	1067	1004
2	580	762	557	731
• 19	16			
0	0	-3099	0	-3554
1	616	-1161	385	-1019
2	-225	66	-1653	307
• 19	17			
0	0	1645	0	1263
1	2491	-629	2563	-631
2	190	-137	259	-692
• 19	18			
0	0	1278	0	1352
1	-572	1443	-719	1815
2	-1436	438	-1278	390
• 19	19			
0	0	-1654	0	-1878
1	979	-1809	953	-1741
2	-1428	425	-1505	566
• 19	20			
0	0	1291	0	1753
1	1194	-1200	1374	-1660
2	1290	276	1465	313
• 19	21			
0	0	2859	0	3276
1	-502	1339	-726	1792
• 19	22			
0	0	-1272	0	-1544
• 19	23			
0	0	1709	0	1652
1	440	-1446	444	-1457
• 19	24			
1	19	1058	14	738
• 19	25			
1	944	-921	922	-863
• 19	26			
0	0	1390	0	1374
• 20	0			
1	0	-2069	0	-2705
• 20	1			
0	2057	0	2625	0
2	233	2328	185	1829
• 20	2			
0	-3070	0	-3465	0
1	-2382	-2948	-2003	-2480
2	-415	844	-507	1029
• 20	3			
0	3227	0	3649	0
1	-838	-2167	-879	-2274
2	-125	-1045	-135	-1136
• 20	4			
1	429	-2886	401	-2640
2	-1734	-323	-1752	-327
• 20	5			
0	1200	0	736	0
1	1099	-1239	1604	-1112
2	947	1156	835	1019
• 20	6			
1	-2278	-2819	-2461	-3045
• 20	7			
0	3284	0	3177	0
1	1281	-44	1594	-59
2	880	-1709	1039	-2019
• 20	8			
1	1689	-1280	2135	-1617
2	708	794	710	796
• 20	9			
0	4417	0	4089	0
1	-1209	-3074	-1308	-3327
2	1820	1605	2107	1843
• 20	10			
0	4304	0	4666	0
1	-1447	1580	-1609	1735
• 20	11			
1	-890	616	-1243	860
2	757	1015	758	1015
• 20	12			
1	-1875	1331	-1975	1402
2	1154	-210	631	-215
• 20	13			
2	-887	-361	-436	-177
• 20	14			
2	49	-955	49	-967
• 20	16			
0	1807	0	2335	0
2	-277	-968	-169	-555
• 20	17			
0	1653	0	1337	0
2	870	-1922	689	-1522
• 20	18			
1	756	1829	796	1922
• 20	19			
1	-1636	-26	-769	-18
2	909	-177	951	-148
• 20	20			
0	2551	0	2294	0
2	327	-939	321	-760
• 20	21			
1	-297	1927	-236	2005
• 20	22			
1	-794	913	-627	562
• 20	23			
1	-1097	414	-1331	502
• 20	24			
1	1483	994	1424	945
• 20	25			
0	-1544	0	-1392	0
• 20	27			
1	1175	922	1474	1156
• 20	28			
0	-2707	0	-2228	0
• 21	0			
1	0	-1987	0	-2139
2	-1792	0	-1562	0
• 21	1			
0	0	-2734	0	-2967
1	452	-1221	434	-1172
2	379	-1293	485	-1632
• 21	2			
0	0	2998	0	2767
1	1969	-284	2370	-342
2	-269	-930	-127	-700
• 21	3			
0	0	-4264	0	-3782
1	507	1205	563	862
• 21	4			
0	0	2129	0	1946
1	2195	1490	2499	1684
2	1	-954	0	-761
• 21	5			
1	1666	932	820	919
2	-381	-976	-419	-963
• 21	6			
1	754	2158	923	2348
• 21	7			
1	575	-1159	585	-1310
2	-1172	676	-1205	694
• 21	8			
1	1283	-331	1294	-332
2	516	1252	569	1382
• 21	9			
1	-1483	802	-1792	891
• 21	10			
1	1180	-989	1057	-884
• 21	11			
1	1218	-534	1400	-636
2	-963	-1415	-862	-1413
• 21	12			
0	0	2541	0	2559
1	3269	-325	3412	-340
• 21	13			
2	-961	941	-933	917
• 21	14			
0	0	2903	0	2830
1	2053	-79	2475	-94
• 21	15			
0	0	3679	0	3682
1	422	1279	431	1304
2	-75	1245	-79	1348
• 21	17			
0	0	1653	0	1145
• 21	18			
2	782	639	1012	852
• 21	19			
0	0	1469	0	1987
• 21	21			
0	0	1247	0	912
• 21	22			
0	0	1231	0	1337
1	-1377	-506	-1456	-528
• 21	23			
1	-514	1134	-592	1306
• 21	24			
1	415	-897	335	-734
• 21	25			
0	0	2311	0	2004
1	-1362	19	-789	11
• 21	26			
1	-868	580	-929	621
• 22	0			
0	-2284	0	-1928	0
2	1588	0	1362	0
• 22	1			
1	1175	-618	1005	-529
• 22	2			
0	3165	0	2592	0
1	-1362	448	-1367	449
2	1114	367	1121	369
• 22	3			
0	-2238	0	-3169	0
1	-851	1613	-1634	1205
• 22	4			
0	3077	0	2647	0
1	-2665	-1752	-2192	-1915
2	1416	-538	1569	-596
• 22	5			
1	-1466	2187	-1098	2254
2	591	-1019	546	-938
• 22	6			
0	1785	0	2062	0
1	1995	-918	2612	-938
• 22	7			
0	2066	0	2548	0
1	-1498	-570	-1376	-340
• 22	8			
0	2837	0	3474	0
1	-663	-895	-962	-1138
• 22	9			
0	4529	0	4916	0
1	-193	2152	-237	2680
• 22	10			
0	-2852	0	-3309	0
1	219	1989	230	1987
2	423	-996	475	-1098
• 22	11			
1	961	943	953	935
2	-227	-1522	-269	-1218
• 22	12			
1	1648	644	1666	652
• 22	13			
0	-1486	0	-1539	0
1	-915	614	-305	805
• 22	14			
1	-1699	41	-975	32
• 22	15			
1	1228	531	964	417
• 22	16			
1	1627	623	995	633
• 22	17			
1	-818	716	-573	502
• 22	18			
1	905	577	1373	875
• 22	19			
0	-1621	0	-1272	0
• 22	26			
0	-1595	0	-2066	0
• 23	0			
1	0	1099	0	905
• 23	1			
0	0	-2647	0	-2975
1	2154	-589	2627	-475
• 23	2			
0	0	2522	0	2652
2	-952	679	-741	528
• 23	3			
0	0	2265	0	2636
1	753	-1932	799	-1911
• 23	4			
2	701	571	906	975
• 23	5			
0	0	2552	0	2639
• 23	6			
0	0	1277	0	945
1	1039	-1276	836	-1021
• 23	7			
0	0	2763	0	2778
• 23	8			
1	-1552	1	-1469	1
• 23	9			
2	593	989	599	999
• 23	10			
0	0	3349	0	3255
1	-717	1479	-680	1402
2	1159	429	954	323
• 23	12			
0	0	2560	0	2800
• 23	13			
0	0	1475	0	1942
1	-978	-1187	-1238	-1502
• 23	14			
1	-1086	1079	-1096	1089
2	-170	1060	-110	649
• 23	15			
1	-1136	-997	-1448	-1236
• 23	16			
1	-1401	168	-1458	175
• 23	17			
1	-1219	1347	-1618	1761
• 23	18			
1	-970	-971	-943	-951
• 23	19			
1	-1135	-744	-585	-384
• 24	0			
1	0	1740	0	1638
2	-942	0	-715	0
• 24	1			
0	-2692	0	-2285	0
• 24	3			
2	95	-955	94	-948
• 24	4			
1	1519	1606	1494	983
2	1186	595	1226	645
• 24	5			
1	-1414	1583	-2009	1964
2	-1191	540	-947	870
• 24	6			
2	-552	-995	-544	-959
• 24	7			
1	590	1175	396	1801
• 24	9			
2	-919	-55	-1645	-46
• 24	10			
2	-913	14	-823	13
• 24	11			
0	-2747	0	-2255	0
2	-742	518	-651	441
• 24	12			
2	-828	565	-1522	679
• 24	13			
2	-822	-551	-813	-328
• 24	14			
1	1146	-809	989	-556
2	-159	1146	-155	982
• 24	15			
0	-1831	0	-1867	0
1	176	-1219	177	-1227
• 25	1			
0	0	2216	0	1926
2	212	1273	341	1603
• 25	3			
0	0	1951	0	1954
2	-233	954	-398	1065
• 25	4			
0	0	1805	0	1464
1	-1030	-1140	-1085	-1198
2	1292	-5	1412	-5
• 25	5			
1	-1525	563	-1869	669
• 25	6			
2	612	-669	112	-122
• 25	7			
2	1972	524	549	268
• 25	8			
1	-1389	618	-1847	822
• 25	9			
1	-1214	730	-747	425
• 25	10			
1	-1305	38	-1369	37
2	-132	-867	-47	-278
• 25	11			
1	-1262	12	-656	7
2	1952	-172	1035	-169
• 25	12			
2	-493	1067	-366	992
• 25	13			
0	0	-2749	0	-1546
• 25	14			
0	0	-956	0	-1345
• 25	18			
0	0	-1152	0	-1459
• 25	19			
0	0	-1299	0	-1138
• 26	0			
2	-1193	0	-1509	0
• 26	2			
2	-562	1004	-587	979
• 26	4			
0	-2514	0	-1155	0
• 26	6			
0	-1910	0	-2531	0
• 26	7			
1	-26	-1056	-40	-1599
• 26	11			
1	203	-1005	313	-1546
• 26	12			
1	-404	-931	-351	-810
• 26	14			
1	376	-912	356	-937
• 27	1			
1	-1245	-249	-1220	-244
• 27	3			
1	-1559	495	-1552	597
• 28	2			
1	-217	-968	-231	-1119
• 28	4			
1	-198	-965	-213	-1054

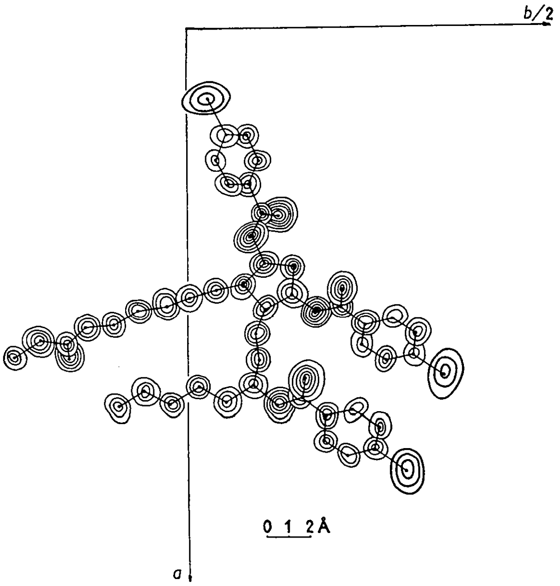


Fig. 4. Composite drawing of the final electron density series. Contours given at intervals of 1 e.Å^{-3} starting with 2 e.Å^{-3} except for the bromine atoms which are contoured at intervals of 5 e.Å^{-3}.

containing a *trans* double bond. The carboxyl group is at the end of a second side chain. The chemistry will be fully discussed elsewhere by Prof. S. Bergström and co-workers.

The X-ray analysis, in addition, gives the stereochemistry of the molecule which would probably have been difficult to determine with conventional chemical methods. Oxidative ozonolysis of PGF_{2-1} yields α-hydroxyheptylic acid with $(\alpha)_D^{23}+9{\cdot}0°$ in sodium hydroxide. According to Baker & Meister (1951) the acid has then the 2D configuration. The absolute configuration of the molecule is thereby known and is given correctly in Fig. 5.

PGF_{1-1} which is formed at the same time as PGF_{2-1} on reduction of PGE_1, which has a carbonyl oxygen instead of the hydroxyl group adjacent to the carboxyl side chain (I) (Bergström *et al.*, 1962*a*), differs from PGF_{2-1} only in the steric position of this hydroxyl group.

The bond distances and angles in the molecule are given in Table 3. The standard deviations were calculated from the diagonal elements of the inverse normal-equations matrix (Ahmed & Cruickshank, 1953; Darlow, 1960). The average values are for bromine: $\sigma(x)=\sigma(y)=0{\cdot}005$ Å, $\sigma(z)=0{\cdot}008$ Å, for oxygen: $\sigma(x)=\sigma(y)=0{\cdot}015$ Å, $\sigma(z)=0{\cdot}025$ Å, and for those carbon atoms which are least accurate: $\sigma(x)=\sigma(y)=0{\cdot}02$ Å, $\sigma(z)=0{\cdot}05$ Å. The accuracy appears

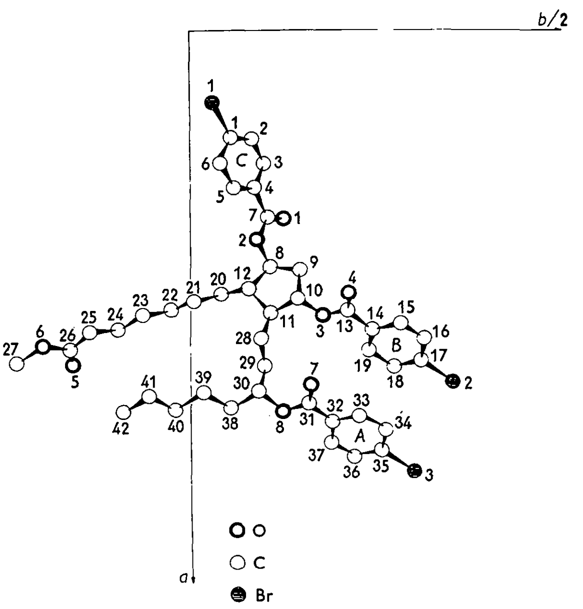


Fig. 5. Spacial diagram of the molecule (correct absolute configuration) with the numbering of atoms indicated.

slightly better if one compares distances and angles with the corresponding generally accepted values but is, of course, still low in a heavily vibrating structure of this complexity. The average values for different classes of distances and angles are given in Table 4.

The molecular packing is illustrated in Fig. 6. The side chains and the benzoate groups project out from the five-membered ring to give a molecule extended in the (001) plane. The two side chains and the bromobenzoate groups *A* and *B* (Fig. 5) are in close contact whereas other molecules can approach the five-membered ring on both sides of group *C*. Similar parts of the molecules are in contact along the short *c*-axis, but this is not possible in other directions and carbon chains have to pack with benzene rings. However, the carbon chains group together as far as possible and alternate with regions of bromobenzoate groups. Some of the most important contacts are shown in Fig. 6 whereas contacts between one molecule and the molecule directly above or below in the *c*-direction are given in Table 5.

The benzene ring, the bromine atom and the carboxyl carbon are in all bromobenzoate groups planar within 0·08 Å. There is an indication that the carboxyl oxygen atoms may be slightly twisted out of the plane (up to 0·15 Å). Benzoate groups *A* and *B* are approximately parallel. Their planes make an angle of 42° with the (001) plane and their twofold axes are tilted 15° to the same plane. The third benzoate

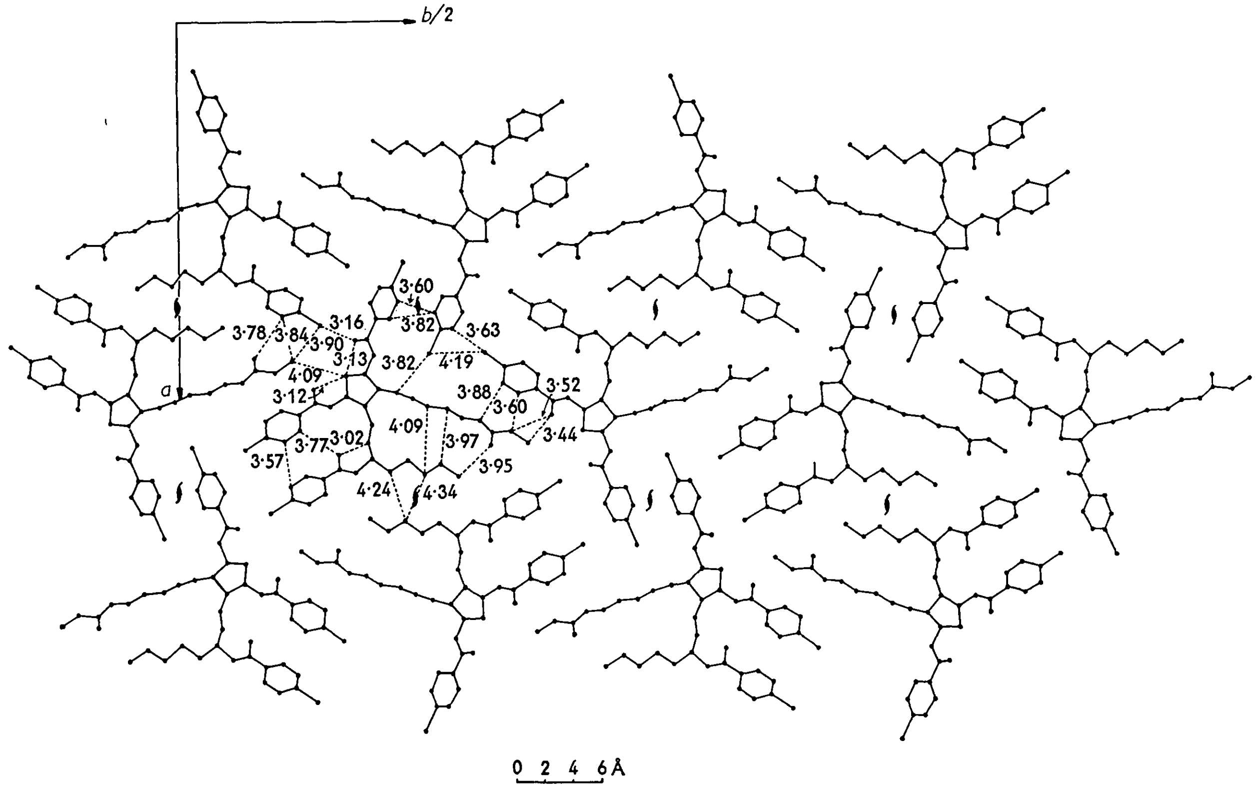


Fig. 6. Molecular arrangement of the *p*-bromobenzoate derivative of the methyl ester of PGF_{2-1} as seen along the *c*-axis with some of the more important contacts shown.

group shows very similar angles but has its diad axis roughly perpendicular to those of the other two groups when the three groups are in packing contact. Most benzene rings in this structure pack with their planes parallel but *C*-rings also make contact with roughly perpendicular planes at screw axes.

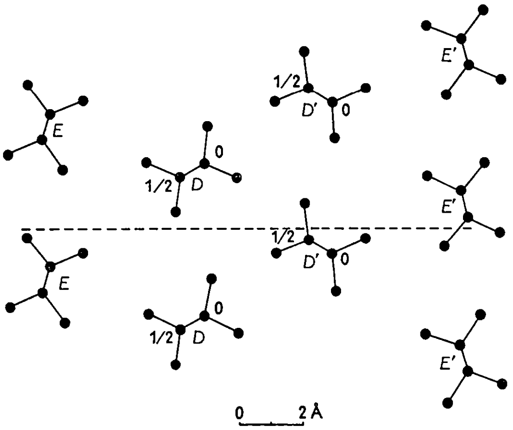
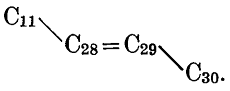


Fig. 7. Schematic representation of the hydrocarbon chain packing as seen along the chain axes. 0 and 1/2 are fractions of the repeat distance (2·55 Å) along a chain. Dotted line indicates the plane $z = 0$.

The hydrocarbon chains are surprisingly regular considering their small length and their packing contacts with benzene rings. Atoms C_{21} to C_{25} are planar within 0·05 Å whereas C_{20} is 0·16 Å off the plane. C_{39} to C_{42} lie within 0·002 Å from a plane with C_{38} at a distance of 0·12 Å. The axes of the two chains are roughly parallel to the (001) plane but are not mutually parallel as the position of the side chains in the molecule prevents them coming into close-packing contact until near their ends. The carbon-chain arrangement is illustrated schematically in Fig. 7. The plane of chain *D* is inclined 28° to the (001) plane and that of chain *E* 76° in the same sense. It is not to be expected that the chain packing should be exactly similar to those found in long-chain structures (*cf.* Abrahamsson *et al.*, 1963) but the general arrangement of *D*-chains resembles very much that of the common orthorhombic type O ⊥.

The atoms of the ester group (C_{25}, C_{26}, O_5, O_6, C_{27}) lie within 0·06 Å or less from a plane, which is twisted 23° from that of the adjoining hydrocarbon chain. A similar angle of twist (19°) is found in methyl stearate (Aleby & von Sydow, 1960).

Four of the atoms (C_8, C_9, C_{10}, C_{12}) of the five-membered ring lie in a plane within 0·07 Å whereas the fifth is at an appreciable distance (0·71 Å) as is usual for such saturated rings. The bonds to the different attached groups are all *trans* relative to the five membered ring (Fig. 5). The bonds C_{30}–O_8 and C_{30}–C_{38} are rotated 45° and 54° respectively out of the plane of the double bonded group


$C_{11}\diagdown C_{28}=C_{29}\diagdown C_{30}$.

I wish to thank Prof. E. Stenhagen and Dr C. Lagercrantz for providing laboratory space for the Crystallography Group in their departments. The technical assistance of Mrs M. Innes and Mr L. Ahlquist and Mr A. Westerdahl is greatfully acknowledged. I also thank Drs O. S. Mills, K. Prout, J. S. Rollett and R. Sparks for use of Mercury programs without which this analysis would not have been performed at the present time. The staff at the Mercury computer of AB Atomenergi, Stockholm have always been very helpful with the calculations.

The work was financially supported by grants from the Swedish Natural Science and Medical Research Councils and by grant A-4006 from the National Institute of Arthritis and Metabolic Diseases, U.S. Public Health Service.

References

Abrahamsson, S. & Maslen, E. N. (1963). *Z. Kristallogr.* In the press.

Abrahamsson, S., Ställberg-Stenhagen, S. & Stenhagen, E. (1963). *Progress in the Chemistry of Fats and Other Lipids*, Vol. 7. Oxford: Pergamon Press.

Ahmed, F. R. & Cruickshank, D. W. J. (1953). *Acta Cryst.* **6**, 385.

Aleby, S. & von Sydow, E. (1960). *Acta Cryst.* **13**, 487.

Baker, C. G. & Meister, A. (1951). *J. Amer. Chem. Soc.* **73**, 1336.

Berghuis, J., Haanappel, IJ. M., Potters, M., Loopstra, B. O., MacGillavry, C. H. & Veenendaal, A. L. (1955). *Acta Cryst.* **8**, 478.

Bergström, S., Krabisch, L., Samuelsson, B. & Sjövall, J. (1962). *Acta Chem. Scand.* **16**, 969.

Bergström, S., Ryhage, R., Samuelsson, B. & Sjövall, J. (1962*a*). *Acta Chem. Scand.* **16**, 501.

Bergström, S. & Sjövall, J. (1960). *Acta Chem. Scand.* **14**, 1693, 1701.

Darlow, S. F. (1960). *Acta Cryst.* **13**, 683.

Dauben, C. H. & Templeton, D. (1955). *Acta Cryst.* **8**, 841.

Euler, U. S. von (1934). *Arch. exptl. Path. Pharmak.* **175**, 78.

Euler, U. S. von (1935). *J. Physiol.* **84**, 21P.

Goldblatt, M. W. (1933). *Chem. & Ind.* **52**, 1056.

Mills, O. S. & Rollett, J. S. (1961). *Computing Methods and the Phase Problem in X-ray Crystal Analysis*, p. 107. Oxford: Pergamon Press.

Thomas, L. H. & Umeda, K. (1957). *J. Chem. Phys.* **26**, 293.