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The Molecular Structure of Trichodermin

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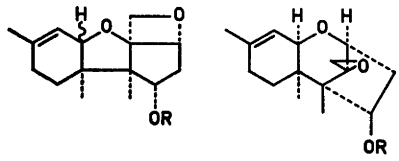
The structure of the antibiotic trichodermin has been determined by X-ray single crystal analysis of trichodermol *p*-bromobenzoate. A new type of ring system was discovered which has later been found to be present in several other natural products. The previously assumed structures of these compounds, which include verrucarol and trichotecin have therefore had to be revised.

Trichodermin ($C_{17}H_{24}O_4$) is a new type of sesquiterpene antibiotic isolated from a soil sample from New Guinea. Godtfredsen and Vangedal have performed extensive chemical studies [1,2] on the antibiotic. They showed that the compound was related to trichotecin,[3,4] and trichodermin was therefore thought to have structure (I) with a four-membered oxygen containing ring suggested to be present in trichotecin.

Some reactions were, however, in conflict with such a structure. At the suggestion of Dr. Godtfredsen we have performed a single crystal analysis in order to establish definitely the molecular structure of the compound. We have earlier published a preliminary paper on the X-ray analysis.[5]



(I) *(II)*

Trichodermin: R = acetyl
Trichodermol: R = H

EXPERIMENTAL

Good single crystals of the trichodermol *p*-bromobenzoate ($C_{22}H_{25}O_4Br$) were kindly provided by Dr Godtfredsen. They are orthorhombic with

$a = 10.69$ Å, $b = 9.24$ Å, and $c = 20.70$ Å

(Cu$K\alpha$-radiation). The space group is $P2_12_12_1$ and there are four molecules per unit cell. Weissenberg photographs were taken for layers 0—4 about the a-axis and for layers 0—2 about [110]. The intensities were estimated visually and corrected for the Lorentz and polarization factors. No absorption correction was made.

STRUCTURE DETERMINATION

The structure was solved by the heavy-atom method. All atoms except hydrogens had been found after 5 cycles of Fourier refinement. The R-value was then 0.22. All Fourier series (including the Patterson synthesis) were scanned for peaks in the computer making possible a short cycle time. The oxygen atoms could be easily differentiated from the carbon atoms from the Fourier maps.

The structure was refined by full matrix least-squares techniques. The hydrogen atoms were included in the structure factor calculations with their expected coordinates and with isotropic temperature factors corresponding to those of the hydrogen carrying heavier atoms. The refinement was continued until the shifts were smaller than one fifth of the standard deviations. The final R-value for the 888 independent reflexions is 0.102.

All calculations were performed on the Datasaab D21 computer with the integrated crystallographic programme system developed at this institute.[6] The formfactors given in the *International Tables for X-ray Crystallography*,

Table 1. Fractional coordinates (with standard deviations) $\times 10^4$ for the heavier atoms of the molecule.

	x	$\sigma(x)$	y	$\sigma(y)$	z	$\sigma(z)$
Br1	1008	(3)	4871	(2)	1585	(1)
O1	1991	(15)	4200	(11)	4871	(5)
O2	2417	(14)	1878	(10)	4546	(4)
O3	3267	(21)	1792	(14)	9802	(5)
O4	1835	(14)	0560	(12)	1373	(4)
C1	1446	(23)	4319	(18)	2455	(6)
C2	1599	(22)	2956	(18)	2611	(6)
C3	1903	(28)	2584	(21)	3265	(7)
C4	1838	(20)	3612	(17)	3702	(6)
C5	1603	(23)	5086	(16)	3557	(7)
C6	3657	(25)	4547	(21)	7912	(7)
C7	2001	(22)	3307	(16)	4428	(6)
C8	2574	(19)	1489	(15)	5208	(6)
C9	1372	(22)	0537	(16)	5475	(6)
C10	3073	(24)	1017	(19)	0414	(6)
C11	1737	(26)	0850	(18)	0684	(6)
C12	3717	(22)	0432	(18)	5267	(8)
C13	0252	(23)	0805	(24)	5101	(8)
C14	3935	(35)	2394	(17)	0398	(8)
C15	1353	(17)	0996	(14)	6199	(6)
C16	2556	(22)	0791	(15)	6540	(7)
C17	0838	(26)	2489	(20)	6287	(7)
C18	0382	(24)	−0140	(18)	6551	(7)
C19	0339	(26)	0424	(20)	7328	(10)
C20	1539	(22)	0627	(20)	7620	(6)
C21	2491	(20)	0821	(15)	7259	(7)
C22	1417	(28)	1001	(25)	8344	(7)

Vol. III (pp. 202–207) were used. The weight assigned to each observation in the least-squares refinement was [7]

$$w = \frac{1}{1 + [(|F_o| - 4|F_{min}|)/3|F_{min}|]^2}$$

RESULTS AND DISCUSSION

The positions for the heavier atoms used in the final calculations of the structure factors are given with standard deviations in Table 1. Allowance was made for anisotropic vibrations by a factor

$$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2lhc^*a^*U_{31} + 2hka^*b^*U_{12})]$$

(Table 2). Table 3 gives the parameters of the hydrogen atoms. Observed and calculated structure factors are listed in Table 4.

A composite drawing of the three-dimensional electron density series based on the final phases is given in Fig. 1. Fig. 2 illustrates the stereochemistry of trichodermol *p*-bromobenzoate. The numbering of atoms is given in Fig. 3.

Table 2. U_{ij}:s × 10^4 for the heavier atoms.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{31}	U_{12} (Å²)
Br1	3017	1016	0577	0195	−0167	0255
O1	1893	0528	0642	0055	−0163	0100
O2	2199	0522	0347	0117	0020	0181
O3	3537	0786	0546	0108	−0201	0174
O4	1921	0695	0543	−0123	0026	0183
C1	2356	0654	0364	0243	0048	0203
C2	1846	0751	0408	−0041	−0056	0162
C3	2375	0947	0534	0122	−0037	−0127
C4	1645	0724	0390	−0054	0114	0197
C5	1878	0557	0687	0122	0177	0083
C6	2411	0843	0550	−0187	0456	0255
C7	1934	0571	0471	−0026	0015	−0037
C8	1709	0438	0494	0173	−0137	0206
C9	2219	0435	0495	0035	0016	0135
C10	2108	0936	0308	0096	0150	−0214
C11	2794	0711	0359	−0134	−0180	0488
C12	1771	0603	0766	0218	0266	−0081
C13	1723	1098	0618	−0029	0241	−0090
C14	3846	0421	0888	−0169	0105	−0132
C15	1158	0545	0452	0109	0133	0249
C16	2232	0443	0672	−0159	−0176	0211
C17	2224	0979	0457	−0078	−0202	0260
C18	2070	0950	0585	0105	0214	−0523
C19	2000	0700	1111	0298	0613	0167
C20	1807	0897	0442	−0078	−0281	0157
C21	2073	0487	0456	−0223	−0126	0191
C22	2897	1284	0502	0229	0398	0857

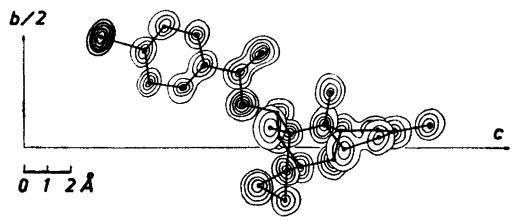


Fig. 1. Composite drawing of the three-dimensional electron density series of trichodermol *p*-bromobenzoate. Contours are given at intervals of 1 e Å^{-3} starting at 1 e Å^{-3} except for the bromine atom which is contoured at intervals of 5 e Å^{-3}.

The X-ray analysis determines the molecular structure of trichodermol as (II). The ring system with the epoxy group is quite different from that of (I) based on the trichotecin structure. The chemical implications of this have been thoroughly discussed by Godtfredsen and Vangedal.[2] The trichodermin ring system seems to be fairly widespread in nature. Godtfredsen and Vangedal suggested a revision of the earlier proposed molecular structures of trichotecin[3,4] and verrucarol.[8] A recent X-ray analysis by McPhail and Sim[9] of the *p*-iodobenzenesulphonate of verrucarin A also confirms the presence of the trichodermin ring system.

Table 3. Fractional coordinates × 10^4 and isotropic temperature factors for the hydrogens of the molecule.

	x	*y*	*z*	*B* (Å^2)
H61	1079	6548	2771	8.1
H51	1622	5909	3934	7.0
H31	2179	1487	3395	8.4
H21	1497	2112	2247	6.5
H161	3433	0628	6282	6.8
H81	2361	2340	5555	5.6
H211	3369	1036	7509	6.0
H121	4001	0053	4790	7.3
H122	4502	0975	5499	7.3
H111	4129	−0934	5408	7.0
H191	−0170	−0381	7609	9.1
H192	−0160	1452	7344	9.1
H181	0730	−1247	6519	8.2
H182	−0544	−0080	6331	8.2
H141	0054	−2290	5448	8.9
H142	1371	−3404	5618	8.9
H221	1560	2159	8412	9.7
H222	2119	0404	8618	9.7
H223	0487	0704	8514	9.7
H171	0762	2728	6802	7.8
H172	−0086	2555	6066	7.8
H173	1460	3271	6059	7.8
H131	0417	0511	4599	8.3
H132	0009	1949	5130	8.3
H133	−0515	0158	5294	8.3

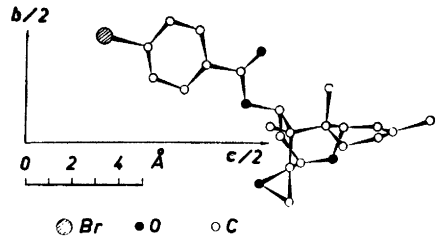


Fig. 2. Stereochemistry of trichodermol *p*-bromobenzoate.

The distances and angles of trichodermol *p*-bromobenzoate are given in Fig. 3 and in Table 5 with the estimated standard deviations. The latter were calculated from the diagonal elements of the inverse least-squares matrix.[10,11] The bond distances and angles show rather large deviations from the generally accepted values, but, considering the standard deviations, there are no anomalies in the structure. The average bond distance between single bonded carbons is 1.55 Å, 1.39 Å for the benzene ring carbons, and 1.46 Å for the C—O distance. The accuracy appears to be much the same as in other bromo derivatives of natural products investigated earlier at this institute, *e.g.* prostaglandin F_{2-1} *p*-bromobenzoate.[12]

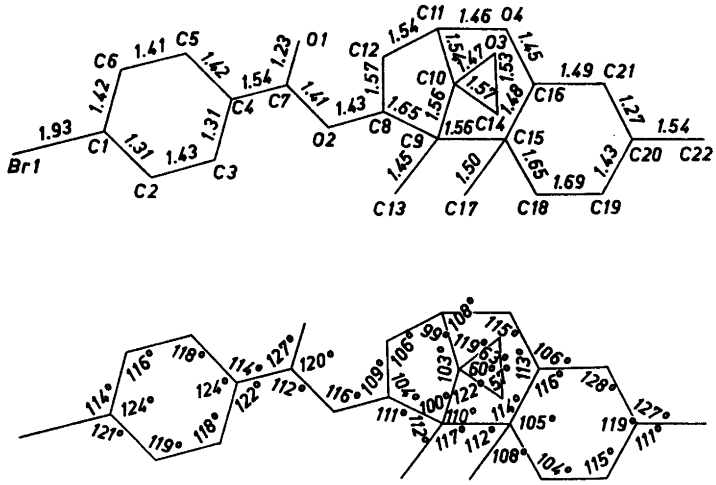


Fig. 3. Bond distances and bond angles for trichodermol *p*-bromobenzoate.

Table 4. Observed and calculated structure factors ($\times$ 100) with phase angles as fractions of one revolution.

h	k	l	Fobs	Fcalc	Fi
0	0	2	1009	854	0.9998
0	0	4	1485	1211	0.9999
0	0	6	14166	16447	1.0000
0	0	8	6466	6853	1.0000
0	0	10	14628	17250	0.5000
0	0	12	3011	3095	1.0000
0	0	16	3691	3696	0.5000
0	0	18	2076	1976	1.0000
0	0	20	1109	960	0.9999
0	0	22	2176	1822	0.5000
0	0	24	1053	1016	0.9999
0	1	1	5590	6595	0.7500
0	1	2	5066	5339	0.2500
0	1	3	1329	926	0.2502
0	1	4	10661	10702	0.2500
0	1	6	4611	5206	0.2500
0	1	7	1211	722	0.7498
0	1	8	4175	4478	0.7500
0	1	9	1962	1584	0.7499
0	1	10	8767	9680	0.2500
0	1	11	1454	1342	0.2501
0	1	12	1228	1327	0.2501
0	1	13	1635	1233	0.2501
0	1	14	5522	5413	0.7500
0	1	16	2990	3067	0.2500
0	1	17	2518	2117	0.7500
0	1	18	3012	2611	0.2500
0	1	20	2786	1680	0.7500
0	1	24	1800	1680	0.2500
0	2	0	19973	20408	1.0000
0	2	1	10427	10417	1.0000
0	2	2	10815	9856	0.5000
0	2	3	2432	2164	0.5001
0	2	4	5160	6507	0.5000
0	2	5	1622	1423	0.9999
0	2	6	8154	10044	1.0000
0	2	8	3435	2950	1.0000
0	2	9	6964	7419	1.0000
0	2	10	6501	7145	0.5000
0	2	12	5295	6178	1.0000
0	2	13	4038	3743	1.0000
0	2	14	3660	3218	1.0000
0	2	15	2280	1950	1.0000
0	2	16	4618	4463	0.5000
0	2	17	1422	1159	0.9999
0	2	18	1706	1534	1.0000
0	2	19	1704	1503	1.0000
0	2	20	1898	1725	1.0000
0	2	21	1493	1159	1.0000
0	2	22	2111	2229	0.5000
0	3	1	1686	1549	0.7499
0	3	2	4437	4802	0.7500
0	3	3	9474	10304	0.7500
0	3	4	3669	3257	0.2500
0	3	5	3286	3408	0.7500
0	3	6	3310	3240	0.2500
0	3	7	1044	866	0.7499
0	3	8	3445	3412	0.7500
0	3	9	4624	4450	0.7500
0	3	10	3956	3885	0.2500
0	3	11	1952	1870	0.7499
0	3	12	2735	2584	0.2500
0	3	13	1668	1386	0.2501
0	3	14	3289	3024	0.7500
0	3	16	1898	1539	0.2501
0	3	20	2277	1740	0.7500
0	3	25	1288	689	0.2501
0	4	0	6113	6599	1.0000
0	4	1	3968	4055	1.0000
0	4	2	5840	5906	0.5000
0	4	3	1649	1533	0.5001
0	4	4	5120	5405	0.5000
0	4	5	1534	1225	0.9999
0	4	6	5917	6450	1.0000
0	4	7	891	753	0.9999
0	4	8	1486	1405	0.5001
0	4	9	3324	3242	1.0000
0	4	10	4584	4792	0.5000
0	4	11	2056	1951	0.5000
0	4	12	3157	3565	1.0000
0	4	13	1996	1423	0.9999
0	4	16	3406	3288	0.5000
0	4	17	2236	1949	0.5000
0	4	18	1106	1008	0.9999
0	5	1	1696	1368	0.2501
0	5	2	6183	6120	0.7500
0	5	3	3415	3581	0.7500
0	5	5	2134	1862	0.7500
0	5	7	994	1123	0.2501
0	5	8	4077	5121	0.7500
0	5	9	1694	1680	0.7500
0	5	11	2077	2216	0.7500
0	5	13	1178	1110	0.2501
0	5	14	1920	1545	0.7500
0	5	15	1118	1075	0.2501
0	5	17	1556	1320	0.7500
0	5	18	1069	981	0.2501
0	6	1	1705	1403	0.9999
0	6	3	1732	1357	0.5001
0	6	4	2661	2580	0.5000
0	6	5	1381	1168	0.9999
0	6	6	3039	3228	1.0000
0	6	8	1892	1779	0.5001
0	6	9	1486	1144	1.0000
0	6	10	2065	1864	0.5000
0	6	11	2326	2232	0.5000
0	6	12	1696	1398	0.9999
0	6	13	1825	1564	1.0000
0	6	16	2164	1979	0.5000
0	7	2	2755	2755	0.7500
0	7	3	3428	3932	0.7500
0	7	4	1496	1329	0.2501
0	7	7	3118	3339	0.2500
0	7	8	1909	1707	0.7500
0	7	9	1361	1233	0.2501
0	7	13	1905	1735	0.2500
0	7	14	1523	1376	0.7500
0	7	15	1043	907	0.2501
0	7	16	999	664	0.2501
0	8	2	1110	921	0.5001
0	8	3	1927	1388	1.0000
0	8	4	3054	2814	0.5000
0	8	6	2373	2214	1.0000
0	8	7	1369	1438	1.0000
1	0	2	7629	8289	0.5000
1	0	3	389	555	0.7496
1	0	4	727	905	0.9998
1	0	5	5312	6786	0.7500
1	0	6	3329	4218	1.0000
1	0	7	3993	4881	0.2500
1	0	8	4524	4780	0.5000
1	0	9	1521	1653	0.2501
1	0	10	839	840	0.9999
1	0	11	4819	5195	0.7500
1	0	12	3822	3494	1.0000
1	0	13	1792	1807	0.2500
1	0	14	2280	2027	0.5000
1	0	15	3371	3342	0.2500
1	0	17	1365	1271	0.7499
1	0	18	2391	2040	1.0000
1	0	21	1906	1795	0.2500
1	1	0	3533	4691	0.2500
1	1	1	6465	5865	0.5678
1	1	2	4954	6464	0.2818
1	1	3	5560	7341	0.9327
1	1	4	4031	4537	0.2230
1	1	5	4567	4649	0.6504
1	1	6	8432	9130	0.8387
1	1	7	5418	6488	0.5525
1	1	8	1684	1060	0.9481
1	1	9	4469	5627	0.9887
1	1	10	1934	1521	0.5138
1	1	11	2812	2881	0.2444
1	1	12	3676	4092	0.7490
1	1	13	3832	4055	0.4316
1	1	14	1601	1530	0.7626
1	1	15	3882	4177	0.0946
1	1	16	1854	1663	0.3826
1	1	17	791	689	0.1564
1	1	18	806	651	0.6840
1	1	19	2745	2888	0.4459
1	1	20	1598	1399	0.7075
1	1	21	774	629	0.0622
1	1	22	1468	1305	0.2566
1	2	0	1194	990	0.2502
1	2	1	5469	6501	0.3167
1	2	2	9222	9990	0.5153
1	2	3	4168	4876	0.3081
1	2	4	2617	2583	0.0033
1	2	5	7594	8290	0.7614
1	2	6	1453	1428	0.6560
1	2	7	4163	4484	0.3021
1	2	8	5623	7127	0.5091
1	2	9	2718	2331	0.2220
1	2	10	2785	2515	0.1109
1	2	11	3098	3573	0.7100
1	2	12	3273	3103	0.9809
1	2	13	487	568	0.4268
1	2	14	2850	2599	0.4928
1	2	15	2555	2489	0.3207
1	2	16	2295	1952	0.0764
1	2	17	1930	1859	0.6688
1	2	18	1716	1362	0.0770
1	2	19	1141	904	0.9509
1	2	20	1120	940	0.5994
1	2	21	1319	1081	0.2291
1	2	22	507	350	0.4107
1	2	23	1201	1245	0.7337
1	3	0	6084	7094	0.7500
1	3	1	5226	4919	0.3591
1	3	2	2997	2786	0.5822
1	3	3	8232	8949	0.9325
1	3	4	811	624	0.2121
1	3	5	2742	2276	0.3266
1	3	6	5961	6799	0.7270
1	3	7	3082	3385	0.4584
1	3	8	1083	888	0.3012
1	3	9	5016	5267	0.9751
1	3	10	2668	2314	0.2582
1	3	11	2388	2081	0.8740
1	3	13	3732	3797	0.4578
1	3	15	2830	2684	0.9403
1	3	16	2754	2932	0.2517
1	3	17	1950	1955	0.7456
1	3	18	1144	890	0.8404
1	3	19	2329	2130	0.4544
1	3	20	775	860	0.6908
1	3	21	737	776	0.8973
1	3	24	1055	571	0.9010
1	4	0	2975	2868	0.2500
1	4	1	3800	3692	0.2401
1	4	2	3053	2864	0.4744
1	4	3	3013	2795	0.5258
1	4	4	2352	2486	0.1311
1	4	5	4785	5411	0.7795
1	4	6	2723	2650	0.8659
1	4	7	2942	2727	0.2667
1	4	8	3393	3679	0.5019
1	4	9	1217	1017	0.1217
1	4	10	1859	1849	0.1031
1	4	11	3536	3519	0.7042
1	4	12	1464	1345	0.8691
1	4	13	2293	2169	0.1667
1	4	14	1654	1387	0.5414
1	4	15	1691	1563	0.3114
1	4	16	1615	1329	0.2467
1	4	17	1982	1840	0.7436
1	4	18	1599	1049	0.0609
1	4	19	778	634	0.1109
1	4	20	1423	1222	0.6173
1	4	21	1301	1034	0.2582
1	5	0	5547	5031	0.7500
1	5	1	2175	2419	0.4842
1	5	2	5955	5881	0.3452
1	5	3	3585	3570	0.9875
1	5	4	3963	4379	0.1988
1	5	5	2301	2336	0.3592
1	5	6	2576	2011	0.9040
1	5	7	2650	2549	0.5581
1	5	8	890	641	0.4041
1	5	9	3615	3771	0.9453
1	5	10	3726	3127	0.2585
1	5	12	2775	2596	0.8923
1	5	13	2780	2686	0.6107
1	5	14	1288	912	0.7845
1	5	15	2602	2182	0.8651
1	5	16	1712	1247	0.3318
1	5	17	1414	1051	0.8423
1	5	18	1477	1320	0.8194
1	5	19	1410	1261	0.4662
1	6	0	1174	1111	0.7499
1	6	1	3174	2878	0.1885
1	6	2	1450	1324	0.9764
1	6	3	1524	1304	0.2718
1	6	4	3861	3206	0.0511
1	6	5	2208	1937	0.7478
1	6	6	2046	1838	0.8351
1	6	7	1998	1891	0.2635
1	6	8	1085	1024	0.5680
1	6	9	2509	2385	0.3797
1	6	10	2557	2275	0.0823
1	6	11	1591	1530	0.6122
1	6	12	1829	1878	0.5969
1	6	13	991	788	0.3487
1	6	14	1837	2199	0.5013
1	6	16	781	804	0.3078
1	6	17	1443	1287	0.6579
1	6	19	945	851	0.0815
1	6	20	862	972	0.5737
1	7	0	3604	3100	0.7500
1	7	1	1510	1174	0.6595
1	7	2	1608	1505	0.3994
1	7	3	2490	2173	0.9783
1	7	4	2926	2712	0.1966
1	7	5	1645	1805	0.3216
1	7	6	960	821	0.6716
1	7	7	1371	1238	0.3635
1	7	8	1384	1428	0.4245
1	7	9	1542	1398	0.9652
1	7	10	2537	2355	0.2394
1	7	11	1619	1398	0.3084
1	7	12	805	798	0.0511
1	7	13	1521	1541	0.3781
1	7	14	777	885	0.5923
1	7	15	981	904	0.0093
1	7	18	1085	1161	0.9066
1	8	0	928	688	0.7499
1	8	1	1468	1128	0.0865
1	8	4	1616	1340	0.3026
1	8	5	1618	1286	0.0458
1	8	6	1718	1535	0.6229
1	8	7	809	655	0.1320
1	8	8	987	766	0.5595
1	8	10	559	412	0.2606
1	8	11	952	979	0.7784
1	8	13	518	457	0.1859
1	8	14	495	456	0.6363
1	9	0	1421	1110	0.7499
1	9	1	977	763	0.6283
1	9	3	973	711	0.0611
1	9	4	968	769	0.0516
1	9	5	1783	1397	0.2675
1	9	6	1099	906	0.8023
1	9	10	874	787	0.2247
1	9	12	927	711	0.9060
2	0	2	5307	5391	0.5000
2	0	3	7501	9861	0.7500
2	0	4	3816	3585	0.5000
2	0	5	608	450	0.2504
2	0	6	1568	1343	0.9999
2	0	7	4504	4727	0.2500
2	0	9	6270	6868	0.7500
2	0	10	2730	2247	1.0000
2	0	11	1600	1663	0.2501
2	0	12	3099	2859	1.0000
2	0	13	6070	6439	0.2500
2	0	15	3092	3029	0.7500
2	0	16	1306	991	0.5001
2	0	17	1804	1420	0.7500
2	0	18	749	701	0.9999
2	0	19	2190	1718	0.2500
2	0	21	876	901	0.7499
2	0	22	676	747	0.5001
2	0	23	1746	1553	0.7500
2	0	24	394	294	0.9998
2	0	25	671	694	0.2501
2	0	26	431	351	0.9998
2	1	0	8182	8199	0.5000
2	1	1	15152	17065	0.0364
2	1	2	7505	8292	0.8580
2	1	3	1778	1778	0.5049
2	1	4	4284	4208	0.0471
2	1	5	7103	7153	0.4688
2	1	6	1530	1307	0.1197
2	1	7	3789	3611	0.9653
2	1	8	4087	3972	0.6441
2	1	9	5074	5594	0.9314
2	1	10	2522	2308	0.9801
2	1	11	5736	6502	0.5334
2	1	12	1902	1684	0.3529
2	1	13	2107	1940	0.9681
2	1	14	1148	1001	0.6938
2	1	15	2041	1574	0.9071
2	1	16	1834	1703	0.5209
2	1	17	3333	3335	0.4817
2	1	18	531	396	0.4952
2	1	19	531	394	0.3105
2	1	20	522	605	0.7986
2	1	21	2074	1978	0.0110
2	1	23	1235	1228	0.4877
2	2	0	4436	4339	1.0000
2	2	1	6557	8527	0.2880
2	2	2	769	813	0.7615
2	2	3	7164	7575	0.7775
2	2	4	4554	4419	0.7919
2	2	5	2200	1954	0.2633
2	2	6	2452	2667	0.0485
2	2	7	5680	6882	0.2371
2	2	8	2720	2708	0.4736
2	2	9	5396	5485	0.7063
2	2	10	2366	2162	0.6183
2	2	11	1584	1473	0.6348
2	2	12	1968	1782	0.9296
2	2	13	3720	4005	0.3030
2	2	14	2166	1914	0.3634
2	2	15	3067	3049	0.6980
2	2	16	1263	1258	0.5987
2	2	17	1054	975	0.5161
2	2	18	2397	2215	0.8439
2	2	19	1057	1032	0.4220
2	2	21	866	822	0.6981
2	2	23	1063	928	0.7217
2	2	24	744	617	0.8462
2	2	25	613	801	0.8477
2	3	0	5593	6363	0.5000
2	3	1	5629	6304	0.9936
2	3	2	1995	1993	0.6175
2	3	3	2105	2012	0.7231
2	3	4	1085	946	0.2370
2	3	5	5254	4954	0.4831
2	3	7	4749	5102	0.0860
2	3	8	3417	3362	0.6267
2	3	9	2627	2391	0.0784
2	3	10	3145	2712	0.0649
2	3	11	4035	3899	0.4775
2	3	12	1215	1246	0.4877
2	3	13	2178	2296	0.0902
2	3	14	1218	930	0.6368
2	3	15	2650	2669	0.2057
2	3	17	2638	2506	0.5357
2	3	18	918	842	0.2531
2	3	20	504	544	0.5689
2	3	21	1784	1665	0.9559
2	3	23	971	895	0.5606
2	4	0	5062	6202	1.0000
2	4	1	2691	3038	0.2111
2	4	2	1614	1594	0.1796
2	4	3	2775	3168	0.8034
2	4	4	2846	2590	0.7195
2	4	5	1120	1184	0.4262
2	4	6	2128	1934	0.0828
2	4	7	4050	3900	0.2459
2	4	8	1444	1202	0.2181
2	4	9	2336	2339	0.7741
2	4	10	1564	1654	0.4321
2	4	12	1376	1007	0.7427
2	4	13	1740	1595	0.2509
2	4	14	2127	1906	0.2264
2	4	15	1488	1335	0.1496
2	4	16	920	764	0.4991
2	4	17	918	868	0.8705
2	4	18	1044	839	0.8600
2	4	19	1430	1398	0.2074
2	4	21	776	738	0.8028
2	4	23	705	700	0.9646
2	4	24	503	412	0.6705
2	4	25	706	694	0.7844
2	5	0	3868	3553	0.5000
2	5	1	3125	3338	0.9696
2	5	2	2059	1998	0.1174
2	5	3	813	861	0.7519
2	5	4	1986	1661	0.2006
2	5	5	3978	3813	0.4515
2	5	6	2005	1478	0.3052
2	5	7	2140	1972	0.0592
2	5	8	2203	1790	0.4522
2	5	9	1521	1223	0.7844
2	5	10	3042	2669	0.1190
2	5	11	3856	4256	0.4548
2	5	12	1648	1651	0.5241
2	5	13	905	888	0.2654
2	5	14	749	647	0.6597
2	5	15	2036	1725	0.8941
2	5	17	1939	1701	0.5269
2	5	18	476	700	0.8625
2	5	20	628	596	0.5761
2	5	21	701	729	0.9720
2	6	0	1462	1324	0.9999
2	6	1	2041	2036	0.1515
2	6	2	2548	2605	0.4818
2	6	3	1780	1755	0.8112
2	6	4	1316	1176	0.6490
2	6	5	1519	1575	0.3695
2	6	6	1546	1320	0.8728
2	6	7	2263	2195	0.2189
2	6	8	999	838	0.2625
2	6	9	1763	1607	0.8470
2	6	10	518	526	0.3485
2	6	11	748	730	0.8138
2	6	12	1298	1247	0.4869
2	6	15	1043	1212	0.8336
2	6	16	1016	1037	0.3701
2	6	18	801	785	0.8590
2	6	19	1081	1120	0.2460
2	6	21	481	574	0.7142
2	7	1	1417	1332	0.1091
2	7	3	1430	1314	0.0433
2	7	4	831	668	0.8243
2	7	5	3341	3175	0.5183
2	7	7	1350	1254	0.9764

Table 4. Continued.

h	k	l	Fobs	Fcalc	F1	h	k	l	Fobs	Fcalc	F1	h	k	l	Fobs	Fcalc	F1	h	k	l	Fobs	Fcalc	F1
2	7	9	1500	1540	0.7631	3	4	0	2815	2879	0.7500	4	1	17	822	760	0.4230	5	0	4	3502	3309	1.0000
2	7	10	1642	1914	0.0051	3	4	1	4492	4824	0.8839	4	1	18	411	471	0.8401	5	0	5	1320	1169	0.2501
2	7	11	1982	1871	0.5435	3	4	2	3077	4660	0.8657	4	1	19	406	615	0.9155	5	0	6	619	510	0.5002
2	7	16	1227	1170	0.9667	3	4	3	1479	1462	0.0076	4	1	20	782	750	0.2570	5	0	7	1365	1339	0.7499
2	7	16	657	517	0.0520	3	4	4	3563	3535	0.0962	4	1	22	484	539	0.2352	5	0	9	262	192	0.2505
2	7	17	616	638	0.4806	3	4	5	2756	3101	0.2111	4	2	0	4283	5066	0.5000	5	0	11	1784	1859	0.2500
2	7	19	359	602	0.1576	3	4	6	872	842	0.2366	4	2	1	1132	1011	0.3727	5	0	13	1193	1073	0.7499
2	7	20	1258	1060	0.4683	3	4	7	1918	1566	0.9198	4	2	2	2810	2644	0.2613	5	0	14	1990	2106	0.5000
2	8	0	1497	1503	1.0000	3	4	8	4008	4115	0.4843	4	2	3	1335	1494	0.6380	5	0	15	1106	1145	0.7499
2	8	1	917	957	0.0545	3	4	9	1288	1327	0.6676	4	2	4	2079	1905	0.0279	5	0	17	1534	1653	0.2500
2	8	2	918	868	0.2192	3	4	10	1594	1590	0.1226	4	2	5	601	514	0.2988	5	1	0	1109	1513	0.2501
2	8	3	1061	766	0.6435	3	4	11	2146	1918	0.3462	4	2	6	2363	2589	0.5592	5	1	1	2013	2310	0.0376
2	8	4	920	690	0.8348	3	4	12	1358	1269	0.0851	4	2	7	1920	1665	0.2145	5	1	2	2833	2079	0.8909
2	8	5	1302	1182	0.3588	3	4	14	2332	2352	0.5216	4	2	8	1748	1683	0.1193	5	1	3	3060	3619	0.5481
2	8	9	739	825	0.7807	3	4	15	778	780	0.7150	4	2	9	1620	1620	0.6316	5	1	4	582	592	0.2671
2	8	10	893	813	0.4513	3	4	16	829	791	0.9073	4	2	10	2806	2698	0.0173	5	1	5	907	781	0.4663
2	8	11	875	867	0.3686	3	4	17	1343	1413	0.3516	4	2	11	925	829	0.0532	5	1	6	700	531	0.2655
2	8	15	695	724	0.8495	3	4	18	999	1013	0.9576	4	2	12	1014	976	0.6194	5	1	7	2766	2944	0.9564
2	8	16	566	633	0.3064	3	4	19	447	476	0.1440	4	2	15	1716	1507	0.9368	5	1	8	1204	948	0.1325
2	9	1	521	674	0.9986	3	4	20	844	907	0.4186	4	2	16	1314	1426	0.4866	5	1	9	1821	1551	0.4692
2	9	4	1030	944	0.0184	3	5	0	2690	3013	0.7500	4	2	17	412	589	0.8430	5	1	11	824	616	0.6028
2	9	5	1444	1210	0.5194	3	5	1	1312	1233	0.8860	4	2	18	409	546	0.7409	5	1	12	546	482	0.3204
2	9	6	505	591	0.5151	3	5	2	1845	1510	0.9967	4	2	19	1007	999	0.1473	5	1	13	1521	1576	0.0143
2	9	7	708	864	0.0952	3	5	4	1595	1654	0.2041	4	2	20	967	866	0.4369	5	1	14	925	924	0.3243
2	9	9	476	573	0.9565	3	5	5	1446	1464	0.1389	4	2	22	574	713	0.0239	5	1	15	496	385	0.2938
2	9	11	443	624	0.2992	3	5	6	2777	2916	0.6832	4	3	0	1024	842	0.9999	5	1	16	506	635	0.6808
3	0	2	8034	9493	0.5000	3	5	7	1465	1300	0.9853	4	3	1	2914	2895	0.9871	5	1	17	620	643	0.2656
3	0	3	666	537	0.7497	3	5	9	615	564	0.5701	4	3	2	2844	2532	0.1873	5	1	19	596	581	0.0266
3	0	4	289	370	0.9995	3	5	10	1182	1160	0.2520	4	3	3	2673	2742	0.2196	5	2	0	850	801	0.7499
3	0	5	1848	1671	0.2501	3	5	11	2319	2550	0.1750	4	3	4	2265	2746	0.7067	5	2	1	3168	3246	0.8305
3	0	6	1182	1150	0.9999	3	5	12	1927	1881	0.5983	4	3	5	2782	2969	0.6034	5	2	2	1821	1147	0.7632
3	0	7	1406	1218	0.7499	3	5	13	1194	1147	0.1041	4	3	6	1359	1319	0.7269	5	2	4	1537	1404	0.9037
3	0	8	6288	7729	0.5000	3	5	14	1972	1666	0.4514	4	3	7	868	863	0.9538	5	2	5	1810	1961	0.1331
3	0	9	4677	5008	0.7500	3	5	16	444	480	0.1497	4	3	8	2206	2184	0.1323	5	2	6	590	524	0.4888
3	0	10	2169	1571	0.9999	3	5	17	1218	1156	0.3121	4	3	9	1344	1147	0.8176	5	2	7	2051	1926	0.7745
3	0	11	1390	1349	0.2501	3	5	18	884	916	0.6669	4	3	10	1407	1238	0.7878	5	2	9	970	897	0.6919
3	0	12	1738	1473	0.9999	3	5	19	591	649	0.1453	4	3	11	1939	1928	0.4861	5	2	10	886	688	0.8439
3	0	14	1581	1525	0.5000	3	5	21	876	841	0.6459	4	3	12	1744	1890	0.7164	5	2	11	1602	1526	0.2509
3	0	15	2950	3173	0.7500	3	6	1	1598	1444	0.8218	4	3	13	2172	2426	0.7593	5	2	12	816	718	0.1398
3	0	16	1485	1450	1.0000	3	6	2	2085	2016	0.4638	4	3	14	1284	1433	0.1623	5	2	13	1289	1283	0.9062
3	0	17	1639	1734	0.7500	3	6	3	1270	1205	0.6393	4	3	16	1323	1556	0.8905	5	2	14	601	683	0.3779
3	0	18	1266	1173	0.9999	3	6	4	1883	2071	0.0730	4	3	17	760	792	0.5141	5	2	15	709	750	0.6185
3	0	20	1398	1338	0.5001	3	6	5	1229	1013	0.1302	4	3	18	1043	947	0.6693	5	2	16	358	599	0.8672
3	0	21	1095	1140	0.7499	3	6	7	1484	1468	0.5047	4	3	20	371	411	0.5796	5	2	17	898	922	0.2260
3	1	0	6007	6310	0.7500	3	6	8	1469	1471	0.4374	4	4	0	3904	3738	0.5000	5	3	0	661	657	0.7499
3	1	1	5161	5008	0.4538	3	6	9	1314	1278	0.7383	4	4	1	737	506	0.7893	5	3	1	999	996	0.9054
3	1	2	6084	5729	0.3000	3	6	10	1720	1668	0.0228	4	4	2	1445	1261	0.2490	5	3	2	1433	1422	0.7562
3	1	3	3543	3978	0.1741	3	6	11	476	547	0.2280	4	4	3	2135	1915	0.7066	5	3	3	1747	1667	0.5187
3	1	4	4178	4485	0.2156	3	6	12	1833	1841	0.0660	4	4	4	778	669	0.5933	5	3	4	1119	1171	0.8435
3	1	5	2487	2080	0.4779	3	6	13	956	953	0.0611	4	4	5	1060	926	0.1789	5	3	5	843	838	0.1595
3	1	6	4759	5096	0.7008	3	6	14	1159	1210	0.5625	4	4	6	2812	2849	0.5768	5	3	7	1858	1679	0.9912
3	1	7	1517	1330	0.4271	3	6	16	899	902	0.0200	4	4	8	1473	1413	0.2656	5	3	8	584	614	0.0795
3	1	8	1829	1741	0.3778	3	6	17	1052	1197	0.3621	4	4	9	1920	1612	0.6703	5	3	9	1489	1465	0.4069
3	1	9	3004	2811	0.4913	3	6	18	807	839	0.9833	4	4	10	1719	1698	0.0510	5	3	10	582	468	0.0035
3	1	10	4331	4019	0.2386	3	7	0	2046	1437	0.7499	4	4	11	1145	1156	0.2166	5	3	12	476	509	0.1883
3	1	11	902	794	0.1527	3	7	1	793	723	0.8894	4	4	12	1178	954	0.5614	5	3	13	980	884	0.9929
3	1	12	2883	2605	0.7792	3	7	2	919	747	0.8460	4	4	13	1206	1355	0.2919	5	3	14	707	611	0.2347
3	1	13	2227	2025	0.5835	3	7	3	653	383	0.6933	4	4	14	667	688	0.4704	5	3	15	900	870	0.9351
3	1	14	1294	1168	0.6604	3	7	4	1656	372	0.4451	4	4	15	824	1039	0.8604	5	3	17	353	491	0.3785
3	1	15	2434	2318	0.6379	3	7	5	2227	2300	0.2040	4	4	16	1231	1427	0.0748	5	3	18	485	548	0.4792
3	1	16	3432	2988	0.1902	3	7	6	1333	1518	0.7355	4	4	19	646	570	0.1635	5	3	19	655	617	0.9786
3	1	18	957	949	0.7075	3	7	8	954	963	0.0401	4	5	1	932	858	0.0400	5	4	0	1242	1171	0.2501
3	1	19	951	921	0.0192	3	7	9	476	449	0.7818	4	5	2	1582	1311	0.1886	5	4	1	1731	1846	0.6781
3	1	20	928	999	0.7948	3	7	10	478	239	0.1406	4	5	3	2081	1837	0.9557	5	4	2	469	516	0.2685
3	1	22	1326	1020	0.2688	3	7	11	476	642	0.1810	4	5	4	1697	1476	0.8971	5	4	3	1452	1149	0.5742
3	1	25	787	773	0.1243	3	7	12	664	795	0.7513	4	5	5	493	686	0.5766	5	4	4	901	715	0.8384
3	2	0	2103	2347	0.2501	3	7	13	797	790	0.9241	4	5	6	1807	1596	0.7429	5	4	5	1380	1393	0.2433
3	2	1	3574	3637	0.8200	3	7	15	606	617	0.7067	4	5	7	1507	1425	0.9877	5	4	6	507	477	0.0517
3	2	2	3735	4282	0.3595	3	8	1	478	395	0.9397	4	5	8	1060	969	0.7414	5	4	7	906	757	0.7667
3	2	3	1290	1118	0.8142	3	8	2	899	905	0.4707	4	5	9	768	745	0.9165	5	4	8	786	773	0.1041
3	2	4	5724	6116	0.1568	3	8	3	829	980	0.4978	4	5	10	1201	1191	0.8266	5	4	9	559	484	0.7130
3	2	5	3749	4385	0.2859	3	8	4	1539	1672	0.9605	4	5	13	1520	1563	0.8454	5	4	10	979	1030	0.7883
3	2	6	2465	2165	0.1001	3	8	5	1104	1190	0.2103	4	5	17	670	667	0.4557	5	4	11	985	1018	0.1687
3	2	7	1531	1256	0.9624	3	8	6	826	902	0.9352	4	5	20	545	679	0.2480	5	4	13	1066	1235	0.9756
3	2	8	4642	4661	0.4174	3	8	10	792	826	0.0468	4	6	0	523	457	0.5009	5	4	14	716	699	0.1713
3	2	9	2231	2011	0.7800	4	0	1	3426	4198	0.2500	4	6	1	931	946	0.2842	5	4	15	715	819	0.7292
3	2	10	2677	2275	0.0336	4	0	2	3420	4021	1.0000	4	6	2	1425	1424	0.1196	5	4	17	343	500	0.1538
3	2	11	1230	1100	0.2630	4	0	3	463	353	0.2504	4	6	3	1061	1110	0.6955	5	5	0	1234	1089	0.2501
3	2	12	1041	941	0.0783	4	0	4	3878	4047	1.0000	4	6	4	1218	1051	0.9022	5	5	1	520	244	0.1822
3	2	13	772	874	0.2772	4	0	5	2978	2175	0.2501	4	6	5	886	985	0.5946	5	5	3	1171	1034	0.5618
3	2	14	3473	3729	0.5129	4	0	6	1332	1384	0.5001	4	6	6	1839	1688	0.4970	5	5	4	965	997	0.6685
3	2	15	2842	2695	0.8028	4	0	7	1455	1227	0.2501	4	6	8	1133	1211	0.2775	5	5	5	548	371	0.0411
3	2	16	1172	1146	0.9220	4	0	8	906	758	0.5001	4	6	9	1147	1310	0.5836	5	5	7	830	864	0.8195
3	2	20	1373	1560	0.4762	4	0	9	2300	2067	0.7500	4	6	11	713	673	0.7941	5	5	8	337	417	0.3105
3	2	24	912	954	0.9820	4	0	10	2528	2659	1.0000	4	6	12	1056	1256	0.5621	5	5	9	1417	1456	0.5077
3	3	0	2301	2115	0.7499	4	0	11	3201	3117	0.2504	4	6	13	408	496	0.3620	5	5	10	947	1038	0.7008
3	3	1	1959	1739	0.7013	4	0	12	1485	1264	0.5001	4	6	14	987	1077	0.4030	5	5	13	358	489	0.9508
3	3	2	4378	4857	0.1749	4	0	15	1435	1375	0.7499	4	6	16	945	991	0.9792	5	5	14	355	310	0.9028
3	3	3	1909	1596	0.4033	4	0	19	741	863	0.2501	4	7	1	567	431	0.8262	5	5	15	698	883	0.5686
3	3	4	4557	5290	0.2585	4	0	23	804	436	0.2501	4	7	2	1012	1102	0.8397	5	6	0	998	989	0.9501
3	3	5	3601	3150	0.3073	4	1	0	2865	2754	0.2000	4	7	3	1016	989	0.3941	5	6	1	1071	1145	0.7569
3	3	6	3227	3780	0.6820	4	1	1	3613	3616	0.8351	4	7	5	408	571	0.1115	5	6	4	961	869	0.6512
3	3	7	472	446	0.3876	4	1	2	2931	2913	0.3002	4	7	6	819	830	0.4454	5	6	5	1523	1564	0.2717
3	3	8	1197	1191	0.4287	4	1	3	1653	1454	0.7717	4	7	7	712	555	0.9588	5	6	6	347	550	0.2096
3	3	9	1901	1795	0.5455	4	1	4	4336	4496	0.7351	4	7	8	1037	985	0.7768	5	6	7	351	492	0.4121
3	3	10	2175	2135	0.2907	4	1	5	4781	4674	0.5883	4	7	11	572	605	0.3225	5	6	8	501	508	0.2964
3	3	11	2090	1994	0.2401	4	1	6	1302	1042	0.5959	4	7	12	562	598	0.4618	5	6	10	716	689	0.7066
3	3	12	2858	2934	0.6730	4	1	7	1782	1674	0.0363	4	7	13	773	931	0.0033	5	6	11	506	539	0.3319
3	3	13	803	723	0.0836	4	1	8	2977	2902	0.2721	4	8	0	672	619	0.5001	5	6	12	355	459	0.5772
3	3	14	2053	1780	0.5859	4	1	9	1175	891	0.2882	4	8	3	671	810	0.7110	5	7	3	617	675	0.5500
3	3	15	1145	1096	0.7179	4	1	10	1529	1446	0.6196	4	8	4	711	758	0.9100	5	7	4	505	561	0.8135
3	3	16	1289	1208	0.2459	4	1	11	2577	1988	0.4662	4	8	5	409	305	0.8640	5	7	5	358	326	0.8392
3	3	17	957	799	0.1416	4	1	12	1946	1859	0.7763	4	8	6	1024	823	0.5627	5	7	6	358	439	0.1821
3	3	18	1195	1059	0.7483	4	1	13	895	887	0.9074	4	8	10	564	561	0.9446	5	7	7	620	837	0.7901
3	3	19	656	642	0.0706	4	1	14	3228	3790	0.2557	5	0	1	472	604	0.7498	5	7	9	501	558	0.5259
3	3	20	445	537	0.6626	4	1	15	1346	1447	0.0621	5	0	2	910	654	0.5002	5	7	10	350	466	0.5643
3	3	22	964	1039	0.2547	4	1	16	1020	915	0.9395	5	0	3	2452	2016	0.2501	5	7	12	335	399	0.5857

Table 5. Bond lengths and bond angles with standard deviations for the heavier atoms of the molecule.

	Bond length (Å)	σ (Å)
Br1—C1	1.93	(0.02)
O1—C7	1.23	(0.02)
O2—C7	1.41	(0.02)
O2—C8	1.43	(0.02)
O3—C10	1.47	(0.02)
O3—C14	1.53	(0.03)
O4—C11	1.46	(0.02)
O4—C16	1.45	(0.03)
C1—C2	1.31	(0.03)
C1—C6	1.42	(0.03)
C2—C3	1.43	(0.03)
C3—C4	1.31	(0.03)
C4—C5	1.42	(0.03)
C4—C7	1.54	(0.02)
C5—C6	1.41	(0.03)
C8—C9	1.65	(0.03)
C8—C12	1.57	(0.03)
C9—C10	1.56	(0.03)
C9—C13	1.45	(0.04)
C9—C15	1.56	(0.02)
C10—C11	1.54	(0.04)
C10—C14	1.57	(0.04)
C11—C12	1.54	(0.03)
C15—C16	1.48	(0.03)
C15—C17	1.50	(0.03)
C15—C18	1.65	(0.03)
C16—C21	1.49	(0.03)
C18—C19	1.69	(0.03)
C19—C20	1.43	(0.04)
C20—C21	1.27	(0.03)
C20—C22	1.54	(0.03)

	Angle (°)	σ(°)
C7—O2—C8	116	(1)
C10—O3—C14	63	(2)
C11—O4—C16	115	(2)
Br1—C1—C2	121	(2)
Br1—C1—C6	114	(2)
C2—C1—C6	124	(2)
C1—C2—C3	119	(2)
C2—C3—C4	118	(2)
C3—C4—C5	124	(2)
C3—C4—C7	122	(2)
C5—C4—C7	114	(2)
C4—C5—C6	118	(2)
C1—C6—C5	116	(2)
O1—C7—O2	120	(2)
O1—C7—C4	127	(2)
O2—C7—C4	112	(2)
O2—C8—C9	111	(2)
O2—C8—C12	109	(2)
C9—C8—C12	104	(2)
C8—C9—C10	100	(2)
C8—C9—C13	112	(2)
C8—C9—C15	101	(2)
C10—C9—C13	115	(2)
C10—C9—C15	110	(2)
C13—C9—C15	117	(2)
O3—C10—C9	118	(2)
O3—C10—C11	119	(2)
O3—C10—C14	60	(2)
C9—C10—C11	103	(2)
C9—C10—C14	122	(3)
C11—C10—C14	129	(2)
O4—C11—C10	108	(2)
O4—C11—C12	115	(2)
C10—C11—C12	99	(2)
C8—C12—C11	106	(2)
O3—C14—C10	57	(2)
C9—C15—C16	114	(2)
C9—C15—C17	112	(2)
C9—C15—C18	105	(2)
C16—C15—C17	112	(2)
C16—C15—C18	105	(2)
C17—C15—C18	108	(2)
O4—C16—C15	113	(2)
O4—C16—C21	106	(2)
C15—C16—C21	116	(2)
C15—C18—C19	104	(2)
C18—C19—C20	115	(2)
C19—C20—C21	119	(2)
C19—C20—C22	111	(2)
C21—C20—C22	127	(2)
C16—C21—C20	128	(2)

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REFERENCES

1. Godtfredsen, W. O. and Vangedal, S. *Proc. Chem. Soc.* **1964** 188.
2. Godtfredsen, W. O. and Vangedal, S. *Acta Chem. Scand.* **19** (1965) 1088.
3. Freeman, G. G., Gill, J. E. and Waring, W. S. *J. Chem. Soc.* **1959** 1105.
4. Fishman, J., Jones, E. R. H., Lowe, G. and Whiting, M. C. *J. Chem. Soc.* **1960** 3948.
5. Abrahamsson, S. and Nilsson, B. *Proc. Chem. Soc.* **1964** 188.
6. Abrahamsson, S., Aleby, S., Larsson, K., Nilsson, B., Selin, K. and Westerdahl, A. *Acta Chem. Scand.* **19** (1965) 758.
7. Mills, O. S. and Rollett, J. S. *Computing Methods and the Phase Problem in X-Ray Crystal Analysis,* Pergamon Press, London 1960, p. 107.
8. Gutzwiller, J. and Tamm, Ch. *Helv. Chim. Acta* **46** (1963) 1786.
9. McPhail, A. T. and Sim, G. A. *Chem. Comm.* **15** (1965) 350.
10. Ahmed, F. R. and Cruickshank, D. W. J. *Acta Cryst* **6** (1953) 385.
11. Darlow, S. F. *Acta Cryst.* **13** (1960) 683.
12. Abrahamsson, S. *Acta Cryst.* **16** (1963) 409.

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