1049. *The Crystal and Molecular Structure of Benzoyl(triphenylphosphoranylidene) Methyl Iodide*

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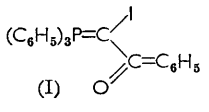
The crystal structure of benzoyl(triphenylphosphoranylidene)methyl iodide has been determined by *X*-ray-diffraction methods: refinement was carried out by an isotropic least-squares procedure with three-dimensional data. There are four molecules in the monoclinic unit cell (space group $P2_1/c$) with dimensions $a = 8{\cdot}248$, $b = 20{\cdot}544$, $c = 13{\cdot}48$ Å, $\beta = 101°\ 21'$. The phosphorus–carbon double-bond length is 1·71 Å, and both the planes containing the carbonyl group and benzoyl ring are twisted from the plane containing the iodine and phosphorus atoms by 12 and 63°, respectively.

The crystal-structure determination of benzoyl(triphenylphosphoranylidene)methyl-iodide (I) was undertaken to obtain a value for the phosphorus–carbon double bond and to ascertain the way in which the overcrowding in the molecule is manifest. If resonance were solely predominant the benzoyl group would be expected to be coplanar with the phosphorus and iodine atoms. Because of the size of the triphenylphosphorus and the benzoyl groups, the preferred orientation of these groups with respect to one another would be *trans*. However, if planarity was retained, the iodine atom would be in close proximity



(I)

TABLE 1

Co-ordinates (Å) and isotropic thermal parameters (Å²) (estimated standard deviations are given in parentheses)

	x	*y*	*z*	*U*
I	−0·154(4)	4·978(4)	1·707(5)	0·063(1)
P	1·121(15)	2·589(16)	3·897(16)	0·042(4)
O	−0·500(36)	3·570(36)	5·628(38)	0·053(10)
C(1)	0·012(67)	1·208(69)	4·152(71)	0·080(21)
C(2)	−1·308(59)	1·200(60)	3·397(63)	0·061(18)
C(3)	−2·123(62)	0·048(66)	3·478(68)	0·068(19)
C(4)	−1·653(71)	−0·920(70)	4·317(76)	0·088(23)
C(5)	−0·381(63)	−1·030(65)	5·036(72)	0·075(21)
C(6)	0·514(65)	0·121(65)	4·881(73)	0·076(21)
C(7)	1·848(49)	2·170(48)	2·471(51)	0·036(14)
C(8)	1·313(49)	1·153(49)	1·594(49)	0·035(14)
C(9)	2·062(69)	1·003(70)	0·447(73)	0·085(23)
C(10)	3·009(71)	1·761(71)	0·329(74)	0·090(24)
C(11)	3·597(65)	2·734(68)	1·108(68)	0·078(21)
C(12)	2·925(60)	2·939(59)	2·258(61)	0·062(18)
C(13)	2·467(50)	2·597(53)	5·346(51)	0·039(14)
C(14)	2·646(66)	3·538(66)	6·474(69)	0·077(21)
C(15)	3·988(59)	3·595(59)	7·446(63)	0·062(18)
C(16)	4·976(74)	2·539(78)	7·257(79)	0·098(25)
C(17)	4·748(65)	1·701(65)	6·300(68)	0·075(21)
C(18)	3·627(57)	1·652(57)	5·318(59)	0·056(18)
C(19)	0·225(48)	4·059(47)	3·732(48)	0·033(14)
C(20)	−0·548(50)	4·391(52)	4·642(51)	0·040(15)
C(21)	−1·588(59)	5·578(59)	4·555(61)	0·064(18)
C(22)	−2·827(53)	5·299(59)	4·716(54)	0·058(15)
C(23)	−3·690(62)	6·516(62)	4·597(64)	0·070(20)
C(24)	−3·048(63)	7·657(66)	4·467(65)	0·072(20)
C(25)	−1·854(88)	8·021(89)	4·294(96)	0·131(33)
C(26)	−0·783(66)	6·786(69)	4·440(71)	0·079(21)

TABLE 2

Calculated and observed structure factors (scale: 100 × absolute)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
0	0	2	-9491	-8693	-798	0	10	4	9832	10664	-832
0	0	4	-20673	-19592	-681	0	10	5	3866	3940	-74
0	0	6	5236	5215	21	0	10	8	-4904	-5516	612
0	0	8	8019	7568	451	0	10	12	3571	2644	927
0	0	12	-5329	-4414	-915	0	11	1	-5493	-6404	911
0	1	1	-4485	-4099	-386	0	11	2	9825	9921	-96
0	1	2	-6833	-7342	509	0	11	5	6206	5724	482
0	1	4	-8082	-8081	-1	0	11	6	-5981	-5905	-76
0	1	6	13365	13052	313	0	11	7	-2982	-3313	331
0	1	7	3757	3847	-90	0	11	10	4463	4820	-357
0	1	9	-2874	-2757	-117	0	11	14	-2904	-1547	-1357
0	1	10	-6268	-5908	-360	0	12	0	5151	5624	-473
0	1	14	3935	3838	97	0	12	2	3920	4009	-89
0	2	0	-17558	-16854	-704	0	12	4	-6973	-7157	184
0	2	1	-13071	-12145	-926	0	12	5	-3013	-2882	-131
0	2	3	-1921	-2396	475	0	12	8	6260	5191	1069
0	2	4	19650	18551	1099	0	13	1	3749	3843	-94
0	2	5	-5088	-4901	-987	0	13	2	-4989	-5449	460
0	2	6	-2479	-3149	670	0	13	3	-3107	4597	1490
0	2	8	-6686	-6768	82	0	13	4	3795	3097	698
0	2	12	4036	3013	1023	0	13	10	-4123	-2993	-1136
0	3	1	1820	1115	705	0	14	0	-5764	-6274	510
0	3	2	12978	12344	634	0	14	3	-5803	-5364	-439
0	3	3	15745	13115	2630	0	14	4	4113	5242	-1129
0	3	5	2625	465	2160	0	14	5	3160	3460	-300
0	3	6	-9096	-9521	425	0	14	7	3107	1209	1898
0	3	7	-5052	-6055	1003	0	15	1	-3160	-3594	434
0	3	8	-2672	-3349	677	0	15	2	4230	5095	-865
0	3	10	7833	6736	1097	0	15	3	5748	6041	-293
0	4	0	5594	5927	-333	0	15	6	-5058	-4972	-86
0	4	1	-2006	-1371	-635	0	16	0	9282	8962	320
0	4	2	-3206	-2528	-678	0	16	2	-3137	-2354	-783
0	4	4	-16178	-16738	560	0	16	4	-3710	-3228	-482
0	4	7	-2904	-2876	-28	0	16	8	3540	2629	911
0	4	8	12211	12367	-156	0	17	7	3238	3486	-248
0	4	10	-4609	-4078	-531	0	18	1	-3335	-3462	123
0	4	12	-3795	-2993	-802	0	18	7	3246	2767	479
0	5	2	-20471	-19314	-1157	0	19	2	4160	3877	283
0	5	3	-2789	-2161	-628	0	20	4	-3238	-1834	-1404
0	5	4	2532	1738	794	1	0	-12	-4730	-5256	526
0	5	6	9073	9917	-844	1	0	-8	14054	14659	-605
0	5	10	-7570	-7205	-365	1	0	-4	-23647	-23043	-604
0	6	0	-15109	-15431	322	1	0	-2	-4114	-5255	1141
0	6	3	-2998	-2907	-91	1	0	0	19592	24004	-4412
0	6	4	13134	13199	-65	1	0	2	-26039	-23666	-2373
0	6	6	-3757	-2768	-989	1	0	4	-10000	-11337	1337
0	6	8	-8096	-8411	315	1	0	8	3422	3951	-529
0	6	9	-3447	-4242	795	1	0	12	-4453	-4725	272
0	7	1	-4740	-4467	-273	1	1	-16	3484	200	3284
0	7	2	10304	10920	-616	1	1	-10	3968	4188	-220
0	7	6	-8414	-8849	435	1	1	-8	3891	3924	-33
0	7	9	-3710	-3199	-511	1	1	-7	5014	4369	645
0	7	10	3471	3528	-57	1	1	-6	-15777	-15386	-391
0	8	0	12188	12958	-770	1	1	-5	-5666	-5405	-263
0	8	1	3680	4784	-1104	1	1	-4	-6615	-5760	-855
0	8	2	-5803	-5133	-670	1	1	-3	15100	12869	2231
0	8	3	2354	2927	-573	1	1	-2	7838	11442	-3604
0	8	4	-7655	-11173	3518	1	1	0	1095	897	212
0	8	5	-2657	-3452	795	1	1	1	-7922	-7744	-178
0	8	8	6128	5229	899	1	1	2	-14976	-14720	-256
0	8	9	2797	2019	778	1	1	4	-5146	-4561	-585
0	8	12	-3610	-3560	-50	1	1	6	18162	17581	581
0	9	1	5315	5016	299	1	1	10	-8115	-8634	519
0	9	2	-12466	-12710	244	1	2	-12	5230	4527	703
0	9	6	8151	8501	-350	1	2	-10	2930	2489	441
0	9	10	-3269	-3648	379	1	2	-8	-9131	-9188	57
0	9	14	3331	1135	2196	1	2	-5	3584	3099	485
0	10	0	-11553	-12039	486	1	2	-4	14654	15088	-234
0	10	1	-5066	-5641	575	1	2	-3	-12369	-10512	-1857

TABLE 2 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
1	2	-1	6268	7215	-947	1	-7	-1	-1945	-1170	-775
1	2	0	-18470	-18364	-2106	1	-7	0	-2791	-2827	36
1	2	1	-8669	-7430	-1239	1	-7	1	-10277	-8465	-1812
1	2	2	-1907	-1508	-399	1	-7	2	10469	11597	-1128
1	2	3	-3937	-3094	-843	1	-7	3	3029	4449	-1420
1	2	4	10961	10601	360	1	-7	5	4815	4223	592
1	2	8	-7407	-6855	-552	1	-7	6	-9915	-11048	1133
1	3	-14	3653	2715	938	1	-7	9	-2775	-1088	-1687
1	3	-10	-7022	-7274	252	1	-7	10	4961	4900	61
1	3	-7	-5138	-5796	658	1	-7	14	-3722	-1444	-2278
1	3	-6	5514	6090	-576	1	8	-12	-4338	-4655	317
1	3	-4	9230	8870	360	1	8	-8	8261	8356	-95
1	3	-3	3092	2632	460	1	8	-7	2838	1516	1322
1	3	-2	-13685	-13740	55	1	8	-5	6376	7482	-1106
1	3	-1	-9616	-13550	3934	1	8	-4	-9815	-10159	344
1	3	0	-15561	-14359	-1202	1	8	-2	-2491	-3115	624
1	3	1	10477	9869	608	1	8	-1	-5014	-4417	-597
1	3	2	15384	15498	-114	1	8	0	8746	9447	-701
1	3	3	-7107	-6444	-663	1	8	1	3891	4490	-599
1	3	4	2883	3396	-513	1	8	2	2791	3904	-1113
1	3	5	2351	1404	957	1	8	3	2952	1983	969
1	3	6	-9454	-10063	609	1	8	4	-7792	-7094	-696
1	3	10	4023	4246	-223	1	8	5	-2637	-3005	368
1	4	-12	-3876	-3603	-273	1	8	8	3568	3967	-399
1	4	-8	7107	7360	-253	1	8	12	-3352	-3609	257
1	4	-6	3523	4143	-620	1	9	-10	3076	3103	-27
1	4	-4	-16862	-17231	369	1	9	-6	-7507	-7655	148
1	4	-3	-13054	-10470	-2584	1	9	-5	-4937	-4545	-392
1	4	-2	5407	4179	1228	1	9	-3	-3745	-4161	416
1	4	-1	-13092	-11100	-1992	1	9	-2	10492	11567	-1075
1	4	0	27601	25226	2375	1	9	-1	6238	7005	-767
1	4	2	4884	4099	785	1	9	2	-7300	-8252	952
1	4	3	4253	4875	-622	1	9	5	-2883	-3292	409
1	4	7	-2661	-2602	-59	1	9	6	8684	8662	22
1	4	8	9669	10556	-887	1	9	9	4130	2811	1319
1	4	13	-2891	-335	-2556	1	9	10	-5038	-4594	-444
1	4	16	3099	1080	2019	1	10	-9	3630	3991	-361
1	5	-14	-4122	-2105	-2017	1	10	-8	-5930	-6182	252
1	5	-10	6061	6421	-360	1	10	-5	-2599	-3312	713
1	5	-9	3592	2558	1034	1	10	-4	8361	8249	112
1	5	-6	-9653	-10583	930	1	10	-3	-2599	-1893	-706
1	5	-2	19078	18141	937	1	10	-1	6731	6931	-200
1	5	-1	-9299	-7805	-1494	1	10	0	-9600	-10691	1091
1	5	0	3122	4071	-949	1	10	1	-3529	-3142	-387
1	5	1	7292	6819	473	1	10	3	-5177	-4387	-790
1	5	2	-26517	-25271	-1546	1	10	4	7454	8457	-1003
1	5	6	8169	8974	-805	1	10	8	-4830	-4846	16
1	5	7	1792	345	1447	1	11	-10	-5161	-5749	588
1	5	10	-5522	-5445	-77	1	11	-6	6022	6783	-761
1	6	-8	-8214	-8914	700	1	11	-5	3614	3345	269
1	6	-6	-3645	-3747	102	1	11	-3	2361	1810	551
1	6	-5	-3314	-3195	-119	1	11	-2	-6477	-7540	1063
1	6	-4	11847	12511	-664	1	11	-1	-4476	-4356	-120
1	6	-3	5199	4544	655	1	11	2	10977	11985	-1008
1	6	-1	4760	4562	198	1	11	4	-2022	-775	-2047
1	6	0	-13292	-12693	-599	1	11	5	5591	5368	223
1	6	1	-4876	-5917	1041	1	11	6	-4892	-5085	193
1	6	2	4461	3120	1341	1	11	10	3692	4062	-370
1	6	3	-4854	-4096	-758	1	12	-7	2891	2167	724
1	6	4	10792	10436	356	1	12	-6	3122	2126	996
1	6	7	5353	4562	791	1	12	-4	-8569	-8824	255
1	6	8	-4799	-4967	168	1	12	0	3576	4513	-937
1	6	9	-3115	-3984	869	1	12	3	2991	2864	127
1	6	12	4795	3592	1207	1	12	4	-6737	-7560	823
1	7	-9	-3099	-3030	-69	1	12	7	-3145	-1935	-1210
1	7	-6	5461	6489	-1028	1	12	8	5861	5302	559
1	7	-5	3446	3087	359	1	13	-10	3992	4044	-52
1	7	-3	4169	3613	556	1	13	-6	-3876	-4033	157
1	7	-2	-18016	-17699	-317	1	13	-4	-3606	-4700	1094

TABLE 2 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
1	13	-3	-3060	-3775	715	2	2	-4	9209	9171	118
1	13	-2	5084	5994	-910	2	2	-2	8378	7085	1293
1	13	1	5061	5996	-935	2	2	-1	4701	3480	1221
1	13	2	-7384	-7567	183	2	2	0	-22625	-20992	-1633
1	13	3	-3992	-5302	1310	2	2	3	-2346	-1280	-1066
1	13	6	3915	2584	1331	2	2	4	11478	10970	508
1	14	-5	-4199	-5355	1156	2	2	5	6268	6109	159
1	14	-4	5000	5950	-950	2	2	6	4674	4206	468
1	14	-3	4653	5785	-1132	2	2	8	-6067	-5864	-203
1	14	0	-5392	-5705	313	2	3	-10	-7950	-6171	-1779
1	14	3	-3937	-4182	245	2	3	-7	-4273	-3981	-292
1	14	4	4114	4443	-329	2	3	-6	7748	7414	334
1	14	7	3753	4464	-711	2	3	-4	6339	4779	1560
1	14	8	-3015	-2950	-65	2	3	-3	11022	9344	1678
1	15	-6	3984	5609	-1625	2	3	-2	-17283	-15582	-1701
1	15	-3	4614	5800	-1186	2	3	-1	-1768	-2002	234
1	15	-2	-4915	-5774	859	2	3	0	-7669	-7614	-55
1	15	1	-4899	-4641	-258	2	3	1	-4596	-2941	-1655
1	15	2	4622	4824	-202	2	3	2	19612	17996	1616
1	15	3	3761	3702	59	2	3	3	-7870	-5997	-1873
1	15	6	-4861	-5243	382	2	3	5	4596	3789	807
1	16	-8	3269	3282	-13	2	3	6	-10760	-10324	-436
1	16	-2	-2722	-2699	-23	2	3	10	4737	3820	917
1	16	-1	-2968	-3694	726	2	3	14	-4202	-2737	-1465
1	16	0	5583	5350	233	2	4	-12	-5288	-4637	-651
1	16	3	3360	4756	-1396	2	4	-8	8160	6656	1504
1	16	4	-3769	-3309	-460	2	4	-7	2940	4007	-1067
1	16	7	-3446	-2686	-760	2	4	-6	10086	8879	1207
1	17	-7	3253	3304	-51	2	4	-4	-22476	-19389	-3087
1	17	-5	-2960	-2661	-299	2	4	-3	3597	1834	1763
1	17	-2	3523	4208	-685	2	4	-2	-4412	-4074	-338
1	17	6	3515	4166	-651	2	4	0	15952	15158	794
1	18	-1	3568	5203	-1635	2	4	1	5743	5881	-138
1	19	-6	3807	1734	2073	2	4	3	5147	4858	289
1	19	-2	-3836	-3260	-576	2	4	4	-9289	-9110	-179
1	19	2	3852	3149	703	2	4	7	-3931	-2627	-1304
1	20	-4	-3984	-2664	-1320	2	4	8	8781	7612	1169
1	25	-6	-4076	-566	-3510	2	4	12	-4229	-3227	-1002
2	0	-12	-4359	-3281	-1078	2	5	-12	-4456	-3167	-1289
2	0	-10	-4718	-3999	-719	2	5	-10	5235	5032	203
2	0	-8	10156	8506	1650	2	5	-6	-13501	-12977	-524
2	0	-6	-4596	-3445	-1151	2	5	-2	7354	7693	-339
2	0	-4	-14577	-13644	-933	2	5	1	4105	3281	824
2	0	0	17319	18370	-1051	2	5	2	-16513	-15056	-1457
2	0	2	6312	5702	610	2	5	3	-3668	-3815	147
2	0	4	-22493	-20200	-2293	2	5	4	4359	3734	625
2	0	8	7039	6447	592	2	5	6	11110	10303	807
2	0	12	-4456	-4569	113	2	5	13	-4053	-1874	-2179
2	1	-11	3545	1769	1776	2	6	-12	4693	3911	782
2	1	-10	7179	5850	1329	2	6	-8	-8834	-7943	-891
2	1	-6	-13046	-12732	-314	2	6	-7	3028	1898	1130
2	1	-4	-2783	-3580	797	2	6	-5	-6986	-6438	-548
2	1	-3	-3379	-2491	-888	2	6	-4	11583	11469	114
2	1	-2	21539	19399	2140	2	6	-1	4876	3786	1090
2	1	-1	-7030	-6850	-180	2	6	0	-9735	-9389	-346
2	1	0	6085	5209	876	2	6	1	-7765	-8323	558
2	1	1	-6067	-4819	-1248	2	6	4	5980	6230	-250
2	1	2	-11793	-10288	-1505	2	6	7	3160	2873	287
2	1	3	5672	4650	1022	2	6	8	-6356	-8022	1666
2	1	4	-8229	-6600	-1629	2	7	-10	-4456	-4265	-191
2	1	6	11022	9884	1138	2	7	-8	-4578	-3293	-1285
2	1	10	-7459	-5941	-1518	2	7	-6	9779	8943	836
2	1	14	3895	1719	2176	2	7	-4	8019	7847	172
2	2	-12	4613	3599	1014	2	7	-3	-2906	-1758	-1148
2	2	-10	5052	3439	1613	2	7	-2	-18396	-17025	-1371
2	2	-8	-10812	-8980	-1832	2	7	-1	5165	3947	1218
2	2	-7	-4631	-4022	-609	2	7	0	3142	1096	2046
2	2	-6	-3295	-2840	-455	2	7	1	-3633	-2112	-1521
2	2	-5	6583	5401	1182	2	7	2	13991	13074	117

TABLE 2 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
2	7	3	3150	3386	-236	2	14	4	5174	4101	1073
2	7	5	4061	2670	1391	2	14	7	5052	4606	446
2	7	6	-8422	-7490	-932	2	14	11	-4097	-854	-3243
2	7	10	4395	4020	375	2	15	-7	-3484	-3418	-66
2	8	-12	-4053	-2911	-1142	2	15	-6	5306	5183	123
2	8	-9	-4456	-4276	-180	2	15	-2	-7118	-6405	-713
2	8	-8	8756	8882	-126	2	15	1	-3475	-3419	-56
2	8	-4	-5052	-5090	38	2	15	3	3597	2678	919
2	8	-3	-6908	-7142	234	2	16	-5	4185	3461	724
2	8	-2	-4674	-5152	478	2	16	0	3983	3755	228
2	8	-1	-7232	-6986	-246	2	16	4	-5533	-5609	76
2	8	0	4737	4787	-50	2	17	-3	-3414	-3444	30
2	8	1	2591	3628	-1037	2	17	-2	5821	4983	838
2	8	2	9394	10648	-1254	2	18	0	-4210	-3549	-661
2	8	4	-12275	-11278	-997	2	18	3	-3677	-3241	-436
2	8	8	5157	4562	595	2	18	6	-3948	-1956	-1992
2	9	-10	4508	3794	714	2	20	-3	-3309	-1095	-2214
2	9	-6	-7933	-7872	-61	2	20	9	3721	606	3115
2	9	-5	-3247	-2968	-279	2	21	5	-3580	-1570	-2010
2	9	-4	-3738	-3689	-49	2	22	-8	-4124	-942	-3182
2	9	-3	-3247	-3796	549	3	0	-10	-6004	-5360	-644
2	9	-2	15419	14651	768	3	0	-8	11707	10833	874
2	9	-1	6224	6448	-224	3	0	-6	3016	2919	97
2	9	0	-2915	-1354	-1561	3	0	-4	-10423	-9325	-1098
2	9	2	-11022	-11427	405	3	0	-2	1575	1294	281
2	9	3	3939	2299	1640	3	0	0	12953	13550	-597
2	9	5	-6470	-6346	-124	3	0	2	5742	5542	200
2	9	6	6285	6206	79	3	0	4	-17264	-14868	-2396
2	9	9	4263	3392	871	3	0	6	3541	1426	2115
2	10	-9	4867	5062	-195	3	0	8	6053	5434	619
2	10	-8	-4788	-4009	-779	3	1	-10	4593	4496	97
2	10	-7	-3695	-2832	-1063	3	1	-6	-6647	-7062	415
2	10	-5	-3843	-4012	169	3	1	-4	-12535	-9988	-2547
2	10	-4	6619	6854	-235	3	1	-3	-2052	-1882	-170
2	10	-2	2879	2772	107	3	1	-2	13031	13691	-660
2	10	-1	6461	6549	-88	3	1	-1	1245	2337	-1092
2	10	0	-8133	-7721	-412	3	1	0	7035	7988	-953
2	10	3	-5419	-4472	-947	3	1	1	-6792	-4015	-2777
2	10	4	8002	7938	64	3	1	2	-8826	-9239	413
2	10	8	-3834	-4064	230	3	1	3	3424	2198	1226
2	11	-6	6461	5925	536	3	1	6	9430	8803	627
2	11	-3	3965	4172	-207	3	1	10	-4904	-5140	236
2	11	-2	-5252	-5573	321	3	2	-8	-10170	-9417	-753
2	11	0	-4219	-5137	918	3	2	-6	-3503	-3258	-245
2	11	1	-6006	-5073	-933	3	2	-4	12963	12388	575
2	11	2	8090	8782	-692	3	2	-3	-2676	-1138	-1538
2	11	4	-3746	-1773	-1973	3	2	-1	-1946	-2244	298
2	11	5	4534	4989	-455	3	2	0	-16176	-15619	-557
2	11	6	-4903	-4784	-119	3	2	1	-2286	-1824	-462
2	11	9	-5095	-2856	-2239	3	2	3	-10578	-7514	-3064
2	12	-6	4351	3681	670	3	2	4	9226	9388	-162
2	12	-4	-8607	-9344	737	3	2	8	-7220	-6134	-1086
2	12	-1	-4964	-5180	216	3	3	-10	-4233	-4233	0
2	12	0	8580	8859	-279	3	3	-8	-4748	-4904	156
2	12	3	3816	3644	172	3	3	-6	12865	12560	305
2	12	4	-5611	-5155	-456	3	3	-4	7970	7818	152
2	12	6	-4009	-3103	-906	3	3	-3	6121	5324	797
2	12	8	5216	5069	149	3	3	-2	-11980	-11025	-955
2	13	-10	3834	4529	-695	3	3	0	-6316	-5869	-447
2	13	-6	-4280	-4096	-184	3	3	2	14268	13414	854
2	13	-2	4132	5262	-1130	3	3	4	5615	5228	387
2	13	1	4334	4246	88	3	3	6	-9391	-8942	-449
2	13	2	-6295	-5204	-1091	3	4	-8	5654	5626	28
2	13	10	-3773	-1412	-2361	3	4	-6	5528	5009	519
2	14	-5	-4456	-5219	763	3	4	-5	-2899	-2025	-874
2	14	-4	4088	4274	-186	3	4	-4	-13002	-12303	-699
2	14	-3	3799	4449	-650	3	4	-3	-3424	-3074	-350
2	14	0	-6207	-4814	-1393	3	4	-2	-10374	-9876	-498
2	14	3	-3773	-4186	413	3	4	-1	-6832	-4856	-1976

TABLE 2 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
3	4	0	16203	14080	2123	3	10	5	3717	4142	-425
3	4	1	6578	6785	-207	3	10	7	4009	2226	1783
3	4	4	-5936	-6252	316	3	11	-6	6647	6752	-105
3	4	7	-3940	-2410	-1530	3	11	-3	4933	5724	-791
3	4	8	6287	5610	677	3	11	-2	-5537	-5412	-125
3	5	-10	4756	4385	373	3	11	1	-5129	-3524	-1605
3	5	-6	-8028	-9300	1272	3	11	2	8924	6471	2453
3	5	-5	-3902	-4905	1003	3	11	6	-5566	-4474	-1092
3	5	-4	4174	4130	44	3	12	-6	5429	5566	-137
3	5	-3	-3785	-3702	-83	3	12	-5	4485	5165	-680
3	5	-2	9265	9051	214	3	12	0	8895	7597	1298
3	5	0	3376	3489	-113	3	13	-7	3795	2409	1386
3	5	2	-12175	-10191	-1984	3	13	-6	-7035	-5976	-1059
3	5	3	4798	2741	2057	3	13	-2	4865	4135	730
3	5	4	-4992	-4588	-404	3	13	1	5157	4016	1141
3	5	5	-3999	-3362	-637	3	13	2	-5488	-5466	-22
3	5	6	9713	8294	1419	3	13	5	-4368	-3107	-1261
3	6	-8	-4641	-5958	1317	3	13	6	4670	4466	204
3	6	-6	-4846	-4467	-379	3	14	-12	4476	1815	2661
3	6	-5	-5722	-4419	-1303	3	14	-5	-5001	-4265	-736
3	6	-4	9596	9585	11	3	14	-4	4485	3193	1292
3	6	-2	6763	6428	335	3	14	-1	5099	4841	258
3	6	-1	11504	8982	2522	3	14	0	-4816	-4076	-740
3	6	0	-9226	-9222	-4	3	14	4	5420	4176	1244
3	6	1	-3707	-3382	-325	3	15	-6	4670	2476	2194
3	6	2	-6490	-6972	482	3	15	-2	-3872	-3337	-535
3	6	4	9527	8736	791	3	15	1	-6393	-5191	-1202
3	6	8	-4174	-4061	-113	3	16	0	4320	2521	1799
3	7	-10	-4388	-4881	493	3	16	3	4271	3111	1160
3	7	-6	4213	4098	115	3	16	4	-5537	-4262	-1275
3	7	-5	3376	3839	-463	3	17	2	-4183	-1946	-2237
3	7	-4	3093	3599	-506	4	0	-16	5545	2250	3295
3	7	-2	-13975	-11983	-1992	4	0	-12	-5300	-3003	-2297
3	7	-1	4116	2661	1455	4	0	-10	-4974	-4084	-890
3	7	1	-7532	-6678	-854	4	0	-8	5901	5231	670
3	7	2	11006	10433	573	4	0	-4	-10062	-9167	-895
3	7	3	-3007	-1694	-1313	4	0	-2	-5199	-5637	438
3	7	4	3201	2521	680	4	0	0	6918	8139	-1221
3	7	5	6773	4816	1957	4	0	2	6787	6273	514
3	7	6	-4145	-3783	-362	4	0	4	-9789	-8464	-1325
3	8	-8	7163	6736	427	4	0	6	-4222	-3198	-1024
3	8	-7	4194	3591	603	4	0	8	6155	4942	1213
3	8	-5	4379	4483	-104	4	0	10	2726	1080	1646
3	8	-4	-10889	-9978	-911	4	1	-10	4974	4844	130
3	8	-2	-4106	-4584	478	4	1	-6	-9656	-7690	-1966
3	8	0	10062	9352	710	4	1	-5	3092	2534	558
3	8	2	6832	6807	25	4	1	-4	-11029	-9273	-1756
3	8	3	3356	2422	934	4	1	-3	-1902	-1128	-774
3	8	4	-12993	-11676	-1317	4	1	-2	10307	11688	-1381
3	8	8	5546	5763	-217	4	1	0	5331	6106	-775
3	9	-10	4564	4381	183	4	1	2	-12129	-10849	-1280
3	9	-6	-4116	-4364	248	4	1	6	5687	4274	1413
3	9	-5	4136	3035	1101	4	1	10	-4659	-3066	-1593
3	9	-3	-4467	-3690	-777	4	2	-10	4080	3388	692
3	9	-2	10540	9414	1126	4	2	-8	-8659	-7187	-1472
3	9	1	3902	4018	-116	4	2	-5	-3326	-2527	-799
3	9	2	-7902	-6906	-996	4	2	-4	9442	9444	-2
3	9	5	-5586	-4749	-837	4	2	-3	3520	3445	75
3	9	10	-4077	-3247	-830	4	2	0	-8343	-8797	454
3	10	-8	-3980	-2424	-1556	4	2	1	4028	2484	1544
3	10	-7	-3590	-4426	836	4	2	2	-4222	-3813	-409
3	10	-6	-4437	-3609	-828	4	2	4	7875	7144	731
3	10	-5	-4154	-3645	-509	4	2	6	3988	2991	997
3	10	-4	10130	9157	973	4	3	-8	-5921	-6161	240
3	10	-3	3746	3512	234	4	3	-6	10409	9647	762
3	10	-1	3065	1495	1570	4	3	-4	2889	2513	376
3	10	0	-8710	-7118	-1592	4	3	-3	3439	3451	-12
3	10	3	-4525	-3306	-1219	4	3	-2	-10327	-11399	1072
3	10	4	8252	6295	1957	4	3	-1	2125	1965	160

TABLE 2 (*Continued*)

h	k	l	F_o	F_c	Δ	h	k	l	F_o	F_c	Δ
4	3	0	-4955	-5111	156	4	10	4	5768	3896	1872
4	3	1	-4100	-2857	-1243	4	10	5	-5494	-1505	-3989
4	3	2	8272	7781	491	4	11	-10	-5586	-2926	-2660
4	3	4	4537	4755	-218	4	11	-6	8822	5990	2832
4	3	6	-7875	-7990	115	4	11	-3	4069	2448	1621
4	4	-8	5403	5330	73	4	11	-2	-5361	-5220	-141
4	4	-4	-5423	-4394	-1029	4	11	1	-3937	-3802	-135
4	4	-2	-6358	-7487	1129	4	11	2	5646	3794	1852
4	4	0	16453	14086	2367	4	11	6	-6326	-3176	-3152
4	4	1	2940	3372	-432	4	12	-2	-4028	-3538	-490
4	4	4	-7611	-5983	-1628	4	12	-1	-3907	-2688	-1219
4	4	7	-3754	-1672	-2082	4	12	0	6461	6178	283
4	5	-10	4985	3791	1194	4	12	4	-5667	-3673	-1994
4	5	-8	6063	6070	-7	4	12	8	6054	2908	3146
4	5	-7	5534	4442	1092	4	13	-8	4883	2227	2656
4	5	-6	-8079	-7079	-1000	4	13	-6	-5698	-5297	-401
4	5	-4	-3061	-3883	822	4	13	-2	6277	4516	1761
4	5	-2	9463	8335	1128	4	13	0	4710	2344	2366
4	5	0	5097	4179	918	4	13	1	4292	2217	2075
4	5	2	-8831	-7261	-1570	4	13	2	-6481	-4365	-2116
4	5	3	4233	1737	2496	4	13	5	-4202	-3177	-1025
4	5	4	-6704	-5856	-848	4	14	0	-5575	-4516	-1059
4	5	5	-4049	-3986	-63	4	14	4	4802	3899	903
4	5	6	8210	8104	106	4	15	2	5617	3547	2070
4	6	-9	5208	2037	3171	4	16	-1	-4384	-2863	-1521
4	6	-8	-5046	-4235	-811	4	17	-11	-5606	-1472	-4134
4	6	-6	-5147	-4525	-622	4	17	-3	-5189	-2671	-2518
4	6	-4	9452	8936	516	4	17	1	6592	2711	3881
4	6	-2	3439	5236	-1797	4	17	2	-4436	-1960	-2476
4	6	-1	3662	3204	458	5	0	-10	-4920	-3566	-1354
4	6	0	-7814	-7410	-404	5	0	-6	10250	9777	473
4	6	1	-4548	-4272	-276	5	0	-4	-5793	-6698	905
4	6	3	2410	729	1681	5	0	0	8643	8374	269
4	6	4	9341	7584	1757	5	0	2	2881	2225	656
4	6	8	-4762	-2746	-2016	5	0	4	-6506	-5396	-1110
4	7	-10	-5026	-3778	-1248	5	1	-6	-5082	-5180	98
4	7	-7	-4873	-4273	-600	5	1	-4	-3657	-4859	1202
4	7	-6	5442	4579	863	5	1	-2	5264	8485	-3221
4	7	-4	7631	6782	849	5	1	0	4941	6768	-1827
4	7	-3	5809	4436	1373	5	1	1	2470	2782	-312
4	7	-2	-8536	-7173	-1363	5	1	2	-8113	-8321	208
4	7	-1	3144	689	2455	5	2	-8	-5740	-5207	-533
4	7	0	-3234	-4056	822	5	2	-4	5373	5785	-412
4	7	1	-3234	-3348	114	5	2	-2	2934	4581	-1647
4	7	2	11579	9649	1930	5	2	0	-4629	-5488	859
4	7	3	-4253	-1725	-2528	5	2	4	6592	6200	392
4	7	5	7386	5987	1399	5	2	5	-4229	-1664	-2565
4	7	6	-4751	-4916	165	5	2	6	4197	2105	2092
4	8	-16	5768	1642	4126	5	3	-8	-4834	-4752	-82
4	8	-8	8648	7326	1322	5	3	-6	7035	6978	57
4	8	-6	4222	4330	-108	5	3	-4	4693	5796	-1103
4	8	-4	-10358	-9200	-1158	5	3	-3	3311	2690	621
4	8	-1	-3835	-3559	-276	5	3	-2	-5524	-6833	1309
4	8	0	3774	3797	-23	5	3	0	-4068	-4167	99
4	8	2	4935	5657	-722	5	3	1	-4596	-4471	-125
4	8	4	-7071	-5114	-1957	5	3	2	4542	4643	-101
4	9	-10	4802	3851	951	5	3	4	4056	4775	-719
4	9	-6	-3957	-3124	-833	5	3	6	-6949	-4570	-2379
4	9	-3	-4517	-3166	-1351	5	4	-10	-5363	-2480	-2883
4	9	-2	7447	7023	424	5	4	-8	6646	6136	510
4	9	1	5381	5310	71	5	4	-4	-5405	-5077	-328
4	9	2	-9310	-7701	-1609	5	4	-2	-8103	-7650	-453
4	9	3	-4701	-5265	564	5	4	0	6171	7416	-1245
4	10	-5	-6522	-5687	-835	5	4	2	4564	4898	-334
4	10	-4	6501	6361	140	5	4	4	-7240	-6388	-852
4	10	-3	3916	3897	19	5	4	6	-4606	-1518	-3088
4	10	0	-5982	-4095	-1887	5	5	-10	4790	2742	2048
4	10	1	5403	1299	4104	5	5	-8	6744	4346	2398
4	10	3	-5748	-4588	-1160	5	5	-6	-7208	-6321	-887

TABLE 2 (*Continued*)

h	*k*	*l*	F_o	F_c	Δ	*h*	*k*	*l*	F_o	F_c	Δ
5	5	-4	-4336	-4788	452	6	2	-12	5427	2219	3208
5	5	-3	-2881	-1697	-1184	6	2	-6	-4129	-3654	-475
5	5	-2	7639	7172	467	6	2	0	-4186	-5637	1451
5	5	3	5179	2419	2760	6	2	1	-2821	-3014	193
5	5	6	6021	4624	1397	6	2	3	3685	1901	1784
5	6	-8	-5038	-4038	-1000	6	3	-4	5335	5360	-25
5	6	-4	7445	7157	288	6	3	-2	-4483	-5572	1089
5	6	-3	-3549	-2529	-1020	6	3	0	-3583	-3461	-122
5	6	-2	5621	5421	200	6	4	0	3787	4459	-672
5	6	-1	4315	4382	-67	6	4	2	4653	5740	-1087
5	6	0	-8967	-9388	421	6	4	4	-6678	-5758	-920
5	6	2	-5815	-5293	-522	6	5	-6	-3890	-2773	-1117
5	6	4	5070	3702	1368	6	5	-2	4550	4676	-126
5	7	-6	4336	4061	275	6	5	4	-4152	-3621	-531
5	7	-2	-6236	-4896	-1340	6	6	-8	-4505	-3919	-586
5	7	0	-3463	-3744	281	6	6	-4	5040	5789	-749
5	7	2	7801	6439	1362	6	6	0	-6086	-5021	-1065
5	7	3	-4336	-2567	-1769	6	6	1	3981	1120	2861
5	8	-7	3916	1636	2280	6	7	-4	4323	3243	1080
5	8	-6	6095	6211	-116	6	7	-3	4174	3364	810
5	8	-4	-6776	-6639	-137	6	7	0	-4061	-5415	1354
5	8	-1	-4003	-2711	-1292	6	7	1	-3549	-1816	-1733
5	8	0	5448	4305	1143	6	7	2	5005	3894	1111
5	8	2	5804	4896	908	6	8	-6	4857	5419	-562
5	8	8	6095	4109	1986	6	8	-4	-7781	-6636	-545
5	9	-6	-5060	-4039	-1021	6	8	-2	-3924	-1883	-2041
5	9	-2	3743	3731	12	6	8	0	4653	3535	1118
5	9	0	3969	3429	540	6	9	-7	4334	3058	1276
5	9	1	5060	4047	1013	6	10	0	-6644	-4851	-1793
5	9	2	-8902	-7457	-1445	6	10	4	5177	2646	2531
5	9	3	-4456	-5248	792	6	11	-2	-5119	-3964	-1155
5	10	-4	4703	3479	1224	6	12	-8	4892	1822	3070
5	10	-2	4229	3953	276	6	13	-3	-4857	-3002	-1855
5	10	0	-5373	-4377	-996	6	13	-1	4323	1767	2556
5	10	4	7025	4871	2154	6	21	-1	5445	807	4642
5	11	-2	-5384	-4437	-947	7	0	0	4350	3845	505
5	11	-1	4121	1720	2401	7	0	4	-4271	-1252	-3019
5	11	0	-4401	-2102	-2299	7	1	-6	-4113	-4030	-83
5	11	1	-6074	-4976	-1098	7	1	2	-3875	-3259	-616
5	12	0	4435	3108	1327	7	2	-1	2971	3202	-231
5	13	-2	4391	4072	319	7	3	-5	3581	1549	2032
5	14	4	5038	2421	2617	7	3	-4	4249	6753	-2504
5	15	-3	4941	3039	1902	7	5	-4	-3559	-4086	527
5	15	-2	-4920	-2587	-2333	7	5	0	4101	3463	638
5	16	-2	-4715	-1247	-3468	7	5	8	2903	1280	1623
5	16	8	4779	1702	3077	7	8	-2	-3955	-3139	-816
5	22	3	-5762	-1469	-4293	7	10	-1	4621	2594	2027
6	0	-16	5813	1074	4739	7	11	2	8317	2170	6147
6	0	-6	4016	5208	-1192	8	1	-6	-4000	-2442	-1558
6	0	-4	-5232	-6393	1161	8	2	-10	4824	2035	2789
6	0	8	5586	3137	2449	8	2	0	-3694	-1389	-2305
6	1	-10	4459	2504	1955	8	6	0	-2677	-1649	-1028
6	1	-6	-4880	-5846	966	8	8	-5	2169	332	1837
6	1	0	5312	6639	-1327	8	9	-9	-3367	-694	-2673
6	1	4	-4675	-4159	-516	8	10	-6	-4316	-2156	-2160

to an *ortho*-hydrogen atom of the benzoyl ring. To minimise this a rotation of the benzoyl ring would be necessary, thus destroying the resonance throughout the molecule and permitting further distortions from planarity to occur.

EXPERIMENTAL

Crystal Data.—$C_{26}H_{20}IOP$, $M = 506{\cdot}3$. Monoclinic, $a = 8{\cdot}248 \pm 0{\cdot}010$, $b = 20{\cdot}544 \pm 0{\cdot}040$, $c = 13{\cdot}488 \pm 0{\cdot}028$ Å, $\beta = 101°\ 21' \pm 15'$. $U = 2234{\cdot}2$ Å^3, D_m = (by flotation) 1·51, $Z = 4$, $D_c = 1{\cdot}505$ g. cm.$^{-3}$, $F(000) = 1008$. Space group $P2_1/c$(C_{2h}^5, No. 14). Cu-K_α

radiation ($\lambda = 1{\cdot}5418$ Å) for cell dimensions, Mo-K_α ($\lambda = 0{\cdot}71069$ Å) for intensity measurements.

Crystals of the compound (m. p. 186—187° decomp.) were obtained as orange plates elongated in the [*a*] direction. Cell dimensions were measured from single-crystal oscillation and Weissenberg photographs. The intensities were collected on a Hilger–Watts linear diffractometer [1] equipped with SrO/ZrO_2 balanced filters. Each reflection in the 0*kl* to 8*kl* layers, to a maximum angle of $\theta = 32{\cdot}5°$, was measured twice, once with the $SrO(\alpha)$ filter in position and once with the $ZrO_2(\beta)$ filter. The time spent on each reflection was 30 secs. Of the 6150 reflections measured, the counts for only 938 reflections were significant (a count was considered significant if it exceeded twice the standard deviation of its measurement), and these were used in subsequent calculations. The intensities were corrected for Lorentz and polarisation effects, but no correction for absorption or extinction was applied. The scattering-factor curves for all atoms used are those given in International Tables, the values for the iodine atom being corrected for anomalous dispersion.[2] All calculations were carried out on an Elliott 803 B computer, with programmes of Daly, Stephens, and Wheatley.[3]

Structure Determination.—The structure was solved in projection down [*a*] from a sharpened Patterson synthesis which served to locate the positions of the iodine and phosphorus atoms. A succession of Fourier approximations allowed the positions of all the remaining light atoms (excluding hydrogens) to be obtained. The *x*-co-ordinates of the iodine and phosphorus atoms were obtained from a three-dimensional sharpened Patterson synthesis. The *x*-co-ordinates for the light atoms were subsequently obtained from the knowledge of the positions of the two heavier atoms and a model of the molecule. The structure was refined by an isotropic least-squares procedure in which the function minimised was $\Sigma w(|F_o| - |F_c|)^2$. Each reflection was weighted as follows: $|F_o| \leqslant F_m$, $w = 0{\cdot}005$; $|F_o| > F_m$, $w = 1/c|F_o|^2$ where c is given by $1/cF_m^2 = 0{\cdot}005$. Reflections, calculated structure factors of which were less than one-third of the observed values, were omitted from the least-square analysis. The number of planes in the final cycle of refinement was 914 and the final values for R and R' * were 0·157 and 0·031, respectively. The final atomic co-ordinates and isotropic thermal parameters together with their estimated standard deviations (in brackets after each parameter) are given in Table 1. Thus 4·978(4) means that the co-ordinate of the atom (4·978 Å) has an estimated standard deviation of 0·004 Å. The calculated and observed structure factors are given in Table 2.

Discussion

The Figure shows the molecule as it appears when projected down [*a*], and also the labelling of the atoms. The bond lengths and bond angles together with their estimated standard deviations are given in Table 3. The bond lengths and angles involving the phosphorus atom and the phenyl rings of the triphenylphosphorus group do not differ significantly from their mean values of 1·79 Å and 107°, respectively. These values are in good agreement with those found in *p*-tolyl triphenylphosphoranylidenemethyl sulphone [4] but the length is rather shorter than that found in triphenylphosphorus (1·828 Å),[5] though not significantly so. The mean values for the C–C distance and the C–C–C angle in the phenyl rings are 1·40 Å and 120°, respectively. The mean planes through the phenyl rings are given in Table 4 and none of the carbon atoms departs significantly from its mean plane. The P=C length of 1·71 Å agrees with that of 1·709 Å found in *p*-tolyl triphenylphosphoranylidenemethyl sulphone.[4] However, the grouping P,C(19),C(20),O exhibits planarity, and the bond lengths indicate that the double bonds are conjugated. The distances, together with those expected if the double bonds were isolated, are given for

* $R' = \Sigma w(|F_o| - |F_c|)^2/\Sigma w|F_o|^2$.

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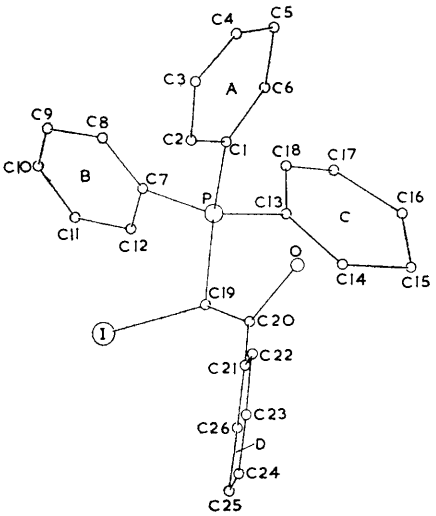

FIGURE 1. The molecule as it appears when projected down *a*, giving the labelling of the atoms

TABLE 3

Bond lengths (Å) and bond angles (°) (estimated standard deviations are given in parentheses)

I–C(19)	2·19(5)	P–C(1)	1·82(7)
O–C(20)	1·28(6)	P–C(7)	1·77(5)
C(19)–C(20)	1·35(7)	P–C(13)	1·77(5)
C(20)–C(21)	1·57(8)	P–C(19)	1·71(5)
C(1)–C(2)	1·39(9)	C(7)–C(8)	1·38(7)
C(2)–C(3)	1·42(9)	C(8)–C(9)	1·50(9)
C(3)–C(4)	1·31(10)	C(9)–C(10)	1·241(0)
C(4)–C(5)	1·34(10)	C(10)–C(11)	1·31(10)
C(5)–C(6)	1·48(10)	C(11)–C(12)	1·46(9)
C(6)–C(1)	1·35(10)	C(12)–C(7)	1·37(8)
C(13)–C(14)	1·45(8)	C(21)–C(22)	1·31(8)
C(14)–C(15)	1·49(9)	C(22)–C(23)	1·48(8)
C(15)–C(16)	1·48(10)	C(23)–C(24)	1·33(9)
C(16)–C(17)	1·26(10)	C(24)–C(25)	1·29(11)
C(17)–C(18)	1·34(9)	C(25)–C(26)	1·62(11)
C(18)–C(13)	1·50(8)	C(26)–C(21)	1·47(9)
C(1)–P–C(7)	107(3)	P–C(1)–C(2)	118(5)
C(1)–P–C(13)	106(3)	P–C(1)–C(6)	121(5)
C(7)–P–C(13)	107(2)		
		P–C(7)–C(8)	121(4)
C(1)–P–C(19)	110(3)	P–C(7)–C(12)	117(4)
C(7)–P–C(19)	115(2)		
C(13)–P–C(19)	112(2)	P–C(13)–C(14)	127(4)
		P–C(13)–C(18)	117(4)
		C(20)–C(21)–C(22)	118(5)
		C(20)–C(21)–C(26)	105(5)
I–C(19)–P	116(2)	O–C(20)–C(19)	115(5)
I–C(19)–C(20)	120(4)	O–C(20)–C(21)	117(4)
P–C(19)–C(20)	120(4)	C(19)–C(20)–C(21)	128(5)
C(6)–C(1)–C(2)	120(6)	C(12)–C(7)–C(8)	122(5)
C(1)–C(2)–C(3)	118(6)	C(7)–C(8)–C(9)	112(5)
C(2)–C(3)–C(4)	120(6)	C(8)–C(9)–C(10)	121(6)
C(3)–C(4)–C(5)	126(7)	C(9)–C(10)–C(11)	131(7)
C(4)–C(5)–C(6)	114(6)	C(10)–C(11)–C(12)	111(6)
C(5)–C(6)–C(1)	121(6)	C(11)–C(12)–C(7)	123(5)
C(18)–C(13)–C(14)	116(5)	C(26)–C(21)–C(22)	137(6)
C(13)–C(14)–C(15)	119(5)	C(21)–C(22)–C(23)	111(6)
C(14)–C(15)–C(16)	115(6)	C(22)–C(23)–C(24)	115(6)
C(15)–C(16)–C(17)	123(7)	C(23)–C(24)–C(25)	137(7)
C(16)–C(17)–C(18)	126(7)	C(24)–C(25)–C(26)	113(7)
C(17)–C(18)–C(13)	120(5)	C(25)–C(26)–C(21)	106(6)

comparison in Table 5. The carbon–iodine distance (2·19 Å) is in accord with a resonance structure, since it is longer than that of 2·09 Å expected [6] for isolated double bonds.

As expected, the benzoyl ring is twisted with respect to the plane containing the carbonyl group by 52°; the latter plane being rotated from the plane containing the phosphorus and iodine atoms. The plane of the benzoyl ring and the planes containing

TABLE 4

Weighted-mean planes in terms of the orthogonal axes, where $x' = x + z\cos\beta$, $y' = y$, $z' = z\sin\beta$, given by the equation $lx' + my' + nz' = p$

	l	m	n	p
Ring A	−0·4650	0·4305	0·7736	4·0062
B	0·5415	−0·6440	0·5405	0·6482
C	−0·5118	−0·6398	0·5733	0·6322
D	0·0574	0·1099	0·9923	4·9364
P,C(19),C(20),O	0·6970	0·4787	0·5339	3·5284
P,C(19),C(20),I	0·7375	0·5789	0·3477	3·1066
C(19),C(20),O,C(21)	0·6424	0·5559	0·5275	3·8708

TABLE 5

Bond lengths (Å) of the P, C(19), C(20), O grouping

Found		Expected		Ref.
P–C(19)	1·71	1·665	P=C	7
C(19)–C(20)	1·35	1·46	(sp^2)C–C(sp^2)	6
C(20)–O	1·28	1·23	C=O	6

the carbonyl group are rotated in the same direction with respect to the plane containing the phosphorus and iodine atoms by 63 and 12°, respectively. The equations of the respective mean planes are given in Table 4.

The shortest van der Waals contact between atoms of neighbouring molecules is from the iodine atom of one molecule to the oxygen atom of another related to the first by (a, $b/2$, $c/2$) at a distance of 3·25 Å (σ = 0·04 Å). This value is just significantly shorter than the sum of the two van der Waals radii for the atoms (3·46 Å),[8] and some interaction between the atoms is indicated. All other intermolecular contacts are greater than 3·5 Å.

I thank Dr. K. W. Ratts of Monsanto Company, St. Louis, for suggesting this problem and supplying the sample; Dr. P. J. Wheatley for his advice and many discussions; and Monsanto Research S. A., Zürich, for providing the funds to enable the work to be carried out.

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[*Received, March 12th*, 1965.]

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