Fig. 1). Nevertheless, the weakness of the terms $(h0l)$ with h odd indicates that the true molecule, as seen in projection, must be very nearly identical in configuration and orientation with the average molecule. The projection suggests that the molecule is probably planar, or very nearly so, and shows that the chlorine atoms are in the *trans* positions; the plane of the molecule may be inclined to the (010) plane at an angle not exceeding 25°.

Further work is now in progress, using all (hkl) reflexions, from which it is hoped to determine accurately the configuration and orientation of the molecules.

References

HARGREAVES, A. & TAYLOR, W. H. (1941). *J. Sci. Instrum.* **18**, 138.

SMARE, D. L. (1942). Thesis for Ph.D. (Manchester).

Acta Cryst. (1948). **1**, 44

The crystal structure of the molecular complex of 4:4′-dinitrodiphenyl with diphenyl.

By J. N. VAN NIEKERK and D. H. SAUNDER. *University of Cape Town, South Africa*

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The structure of this complex seems to be almost identical with the structure of the complex of 4:4′-dinitrodiphenyl with 4-hydroxydiphenyl previously described by one of us (Saunder, 1946). This is confirmed by the very close agreement between the observed F values after allowance has been made for the extra OH group.

The crystals, which grow as pale yellow needles, develop mainly the prism faces {110}, though occasionally the (100) and (001) faces may develop as well. The unit cell dimensions are

$$a = 19{\cdot}9 \text{ A.}, \quad b = 9{\cdot}50 \text{ A.}, \quad c = 11{\cdot}0 \text{ A.}, \quad \beta = 99° 30',$$

and this cell contains two of the complex groups

$$(C_6H_5C_6H_5) \cdot (O_2NC_6H_4C_6H_4NO_2)_3.$$

This may be compared with the dimensions

$$a = 20{\cdot}0 \text{ A.}, \quad b = 9{\cdot}46 \text{ A.}, \quad c = 11{\cdot}1 \text{ A.}, \quad \beta = 99° 39',$$

for the similar complex with hydroxydiphenyl

$$(C_6H_5C_6H_4OH) \cdot (O_2NH_6H_4C_6H_4NO_2)_3.$$

Reflexions of type hkl occur only with $h+k$ even, $h00$ only with h even, and $0k0$ only with k even. The space group may therefore be $C2$, Cm or $C2/m$, and all these space groups are spatially possible. In the case of the complex with hydroxydiphenyl the space group was fixed from spatial considerations as Cm.

Comparative photographs for the two complexes are almost identical, and the thermal vibrations in each produce diffuse reflexions accompanying corresponding spectra.

The $h0l$ spectra were recorded on a Weissenberg photograph taken with a crystal mounted about the b axis. The intensities of these spectra were measured on a microphotometer calibrated against a standard wedge. The values of $F(h0l)$ are compared with the corresponding values of $F(h0l)$ observed for the complex with hydroxydiphenyl (after subtracting the calculated contribution of the OH group) in Table 1. The agreement is excellent.

Assuming the space group $C2/m$, a Fourier projection of the unit cell along b on to the ac plane was made, and the contour diagram thus obtained was found to be closely similar to the corresponding contour diagram for the complex with hydroxydiphenyl, the only significant difference being that there was no peak corresponding to the position of the OH group.

If the space group is either Cm or $C2/m$, it should be noted that, since there are only two 'complex groups' in the unit cell, it is then necessary for the diphenyl molecules to lie completely in the mirror planes, and for the dinitrodiphenyl molecules to lie across the mirror planes, as was found to be the case for the hydroxydiphenyl complex. It should be possible to distinguish between the possible space groups by observing the pyro-electric effect, but we have been unable to obtain single crystals large enough to make satisfactory measurements.

Table 1

$h0l$	D	H	$h0l$	D	H
200	80	72	801	60	69
400	120	109	802	160	146
600	82	93	803	31	59
800	41	46	804	15	24
10.0.0	14	27	805	47	71
14.0.0	17	26	806	21	25
001	25	28	807	23	26
002	27	35	$80\bar{1}$	27	41
003	270	219	$80\bar{2}$	26	43
004	20	22	$80\bar{3}$	79	81
005	29	49	$80\bar{4}$	58	59
006	23	32	$80\bar{5}$	14	
007	20	28	$80\bar{8}$	22	31
201	60	56	8.0.10	24	34
202	74	76	10.0.1	22	35
204	23	24	10.0.2	44	52
205	21	35	10.0.5	22	21
$20\bar{1}$	37	29	10.0.6	23	23
$20\bar{2}$	53	40	$10.0.\bar{1}$	220	197
$20\bar{3}$	240	177	$10.0.\bar{3}$	19	
$20\bar{4}$	36	41	$10.0.\bar{4}$	106	84
$20\bar{5}$	71	59	$12.0.\bar{1}$	39	55
$20\bar{6}$	155	114	$12.0.\bar{5}$	19	20
402	43	32	$12.0.\bar{7}$	33	38
403	70	80	$14.0.\bar{1}$	37	37
404	20	19	14.0.2	36	42
405	20	28	$14.0.\bar{1}$	82	81
$40\bar{1}$	110	88	$14.0.\bar{5}$	27	35
$40\bar{2}$	36	35	16.0.1	33	27
$40\bar{3}$	14	14	$16.0.\bar{1}$	13	16
$40\bar{4}$	44	42	$16.0.\bar{5}$	27	44
$40\bar{5}$	16	21	$16.0.\bar{7}$	37	54
602	120	110			
603	56	62			
604	22	25			
605	15	—			
606	17	—			
$60\bar{1}$	176	120			
$60\bar{2}$	80	68			
$60\bar{3}$	23	24			
$60\bar{6}$	21	32			
$60\bar{8}$	25	28			

$D = F(h0l)$ observed for the diphenyl complex.

$H = F(h0l)$ observed for hydroxydiphenyl complex, and after subtraction of the contribution of the OH group.

Reference

SAUNDER, D. H. (1946). *Proc. Roy. Soc.* A, **188**, 31.