Molecular Structure of One of the 1:2 Adducts from Diphenylsulphur Di-imide and Diphenylketen

By YASUSHI KAI, NORITAKE YASUOKA, NOBUTAMI KASAI,* TORU MINAMI, KAZUNORI YAMATAKA, YOSHIKI OHSHIRO, and TOSHIO AGAWA

(*Department of Applied Chemistry, Faculty of Engineering, Osaka University, Yamadakami, Suita, Osaka, 565, Japan*)

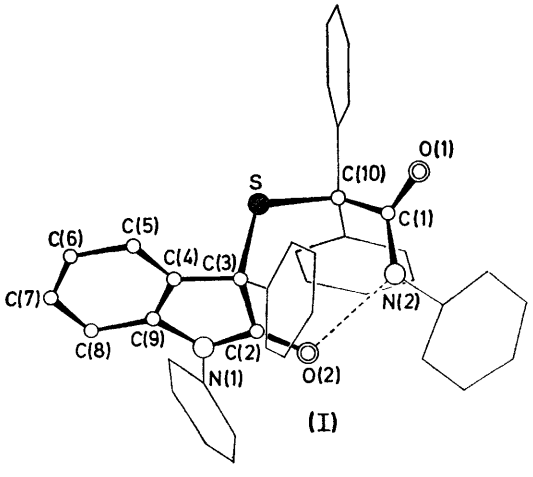
Summary A single crystal *X*-ray diffraction study of one of the 1:2 adducts from diphenylsulphur di-imide and diphenylketen has shown that the structure is 2,3-dihydro-1,3-diphenyl-2-oxoindol-3-yl diphenyl(phenylcarbamoyl)methyl sulphide.

STUDIES on the reaction of sulphur di-imide with diphenylketen have been previously reported.[1] Two types of 1:1 cycloadducts, 1,2,5-thiadiazolidin-4-one and 1-imino-1,2-thiazetidin-3-one, were obtained in the reaction, but no description of the 1:2 adducts has so far been given. By control of the reaction conditions, we have shown that two kinds of 1:2 adducts are formed in the reaction between diphenylsulphur di-imide and diphenylketen. One of them is an unstable product (A) and the other a stable product (B), m.p. 208 °C. On heating (A), (B) is obtained with 2,3,3,5-tetraphenyl-1,2,5-thiadiazolidin-4-one and diphenylketen. By *X*-ray analysis we have shown that (B) has the structure shown in the Figure.

Crystal data: $C_{40}H_{30}O_2N_2S$, Mol. Wt. 602·8; monoclinic, space group $P2_1/a$; $a = 22{\cdot}206(6)$, $b = 11{\cdot}907(2)$, $c = 12{\cdot}027(4)$ Å, and $\beta = 100{\cdot}50(2)°$, $U = 3126$ Å^3; $D_m = 1{\cdot}26$ (flotation method), $D_c = 1{\cdot}28$ g cm^{-3} for $Z = 4$.

The three-dimensional intensity data were collected on a Rigaku on-line controlled single crystal diffractometer with nickel-filtered Cu-K_α radiation. The structure was solved by the symbolic addition method,[2] and then refined by block-diagonal least-squares procedures with anisotropic temperature factors, including isotropic hydrogens ($R = 0{\cdot}056$ for 3030 reflections).

Important bond distances and angles in the molecule are given in the Table.



(I)

FIGURE. *The molecular structure of 2,3-dihydro-1,3-diphenyl-2-oxoindol-3-yl diphenyl(phenylcarbamoyl)methyl sulphide.*

TABLE

Bond distances (Å)		Bond angles (°)	
S–C(3)	1·869(4)	N(1)–C(2)–C(3)	107·6(3)
		C(2)–C(3)–C(4)	101·9(3)
S–C(10)	1·881(4)	C(3)–C(4)–C(9)	109·5(4)
N(1)–C(2)	1·386(5)	C(4)–C(9)–N(1)	109·9(4)
C(2)–C(3)	1·540(6)	C(9)–N(1)–C(2)	110·3(3)
C(3)–C(4)	1·509(6)	N(1)–C(2)–O(2)	125·0(4)
C(4)–C(9)	1·375(6)	C(3)–C(2)–O(2)	127·4(4)
C(9)–N(1)	1·416(6)	C(2)–C(3)–S	108·2(3)
C(2)–O(2)	1·215(5)	C(4)–C(3)–S	100·7(3)
C(10)–C(1)	1·554(6)	C(3)–S–C(10)	115·1(2)
C(1)–O(1)	1·221(5)	S–C(10)–C(1)	111·3(3)
C(1)–N(2)	1·344(5)	C(10)–C(1)–O(1)	120·9(4)
N(2)···O(2)	2·786(4)	C(10)–C(1)–N(2)	114·8(4)
		O(1)–C(1)–N(2)	124·2(4)

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[2] J. Karle and I. L. Karle, *Acta Cryst.*, 1966, **21**, 849.