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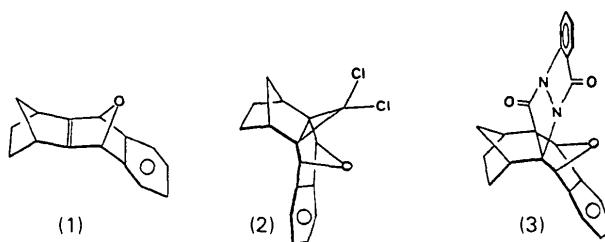
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1,2,3,4,9,10-Hexahydro-9,10-exo-epoxy-1,4-exo-methanoanthracene[†](1) (*syn*-Oxabenzosesquinorbornene), $C_{15}H_{14}O$, and Adducts with Dichlorocarbene (2), $C_{16}H_{14}Cl_2O$, and Anthranilic Acid (3), $C_{23}H_{18}N_2O_3$

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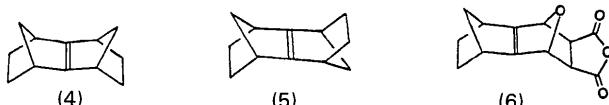
Abstract. (1): $M_r = 210.28$, orthorhombic, $Pna2_1$, $a = 21.552$ (7), $b = 6.503$ (3), $c = 7.652$ (2) Å, $V = 1072.5$ (7) Å³, $Z = 4$, $D_x = 1.302$ g cm⁻³, Mo $K\alpha$, $\lambda = 0.71069$ Å, $\mu = 0.86$ cm⁻¹, $F(000) = 448$, room temperature, $R = 0.046$ for 1026 unique reflections. (2): $M_r = 293.19$, orthorhombic, $P2_12_12_1$, $a = 13.821$ (4), $b = 28.184$ (9), $c = 6.561$ (1) Å, $V = 2556$ (1) Å³, $Z = 8$, $D_x = 1.524$ g cm⁻³, Mo $K\alpha$, $\lambda = 0.71069$ Å, $\mu = 4.96$ cm⁻¹, $F(000) = 1216$, room temperature, $R = 0.060$ for 1795 unique reflections. (3): $M_r = 370.41$, monoclinic, $P2_1/c$, $a = 12.101$ (6), $b = 18.658$ (7), $c = 7.584$ (2) Å, $\beta = 90.26$ (3)°, $V = 1712$ (1) Å³, $Z = 4$, $D_x = 1.437$ g cm⁻³, Cu $K\alpha$, $\lambda = 1.54178$ Å, $\mu = 7.92$ cm⁻¹, $F(000) = 776$, room temperature, $R = 0.043$ for 1897 unique reflections. In (1) the two carbon atoms of the central double bond [1.339 (3) Å] are pyramidalized, and the double-bond system deviates from planarity by 22.1 (2)°. This is the largest deviation yet reported for this type of distortion. In (2) dichlorocarbene has added to the *exo*-face of (1). The two independent molecules have short intramolecular contacts, Cl···O = 2.567 (6) and 2.568 (6) Å and Cl···H = 2.05 and 2.14 Å. Carbon atoms forming the C(2)–C(3) bond in the phenyl ring are slightly pyramidalized but in a direction opposite to that normally observed in sesquinorbornene-type systems. This is attributed to an attractive interaction between the *endo* hydrogens H(6) and H(7) and the π system of C(2) and C(3). The four C(sp²)···H distances in the two independent molecules range from 2.18 to 2.27 Å. Compound (3) is formed by the reaction of (1)



with anthranilic acid. By a yet not understood mechanism an *N*-formylindazolone moiety is formally added to the reactive double bond. The resulting tricyclic fragment is forced through intramolecular contacts to be planar which leads to extensive electron delocalization. The C(2) and C(3) atoms of the phenyl ring are pyramidalized, and the associated π system deviates from planarity by 3.4 (3)°.

Introduction. The variation in reactivity of carbon–carbon double bonds due to the electronic effects of substituents and to perturbations by geometric distortions are, in principle, well understood. However, the study of *syn*- and *anti*-sesquinorbornene, (4) and (5), led to the investigation of some unusual stereo-electronic properties of the π systems (Bartlett, Blakeney, Kimura & Watson, 1980). The π system in the *endo* anhydride of the *anti* isomer (5) is essentially planar in the solid state while the nominally sp² carbon atoms in two derivatives of the *syn* isomer are pyramidalized, and the π system deviates from planarity by 16–18° (Watson, Galloy, Bartlett & Roof, 1981). A similar hinge-like distortion was observed in *syn*-oxasesquinorbornene anhydride (6) (Hagenbuch,

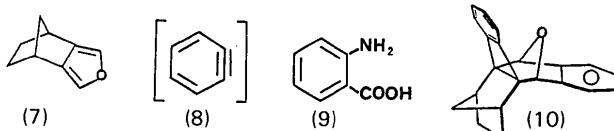
[†](1R*, 4S*, 9S*, 10R*) conformation.



Vogel, Pinkerton & Schwarzenbach, 1981) and several other derivatives (Paquette, Charumilind, Böhm, Gleiter, Bass & Clardy, 1983). The pyramidalization of the carbon atoms of the π system has been attributed to torsional interactions between the bridgehead hydrogen atoms and the allylic bonds (Houk, 1983; Houk, Rondan, Brown, Jorgensen, Madura & Spellmeyer, 1983) and to antibonding hyperconjugative interactions between the π system and σ and σ^* orbitals of the ethylene or the methylene bridges (Gleiter & Böhm, 1983; Vogel, 1983; Spanget-Larsen & Gleiter, 1983). *syn*-Oxabenzosesquinorbornene (1) is of interest because of modifications of the electronic character around the double bond and of the intramolecular steric interactions.

A comparison of the rates of reaction of *syn*-benzo-*sesquinorbornene* and (1) shows that for concerted attack on the central double bond the replacement of CH_2 by O is sterically favorable while polar effects are unfavorable (Bartlett & Combs, 1984). The most striking difference in reactivity occurred upon the addition of dichlorocarbene. In the case of *syn*-benzo-*sesquinorbornene*, treatment with dichlorocarbene for 24 h results in no reaction, while treatment of (1) under similar conditions results in complete reaction within 12 h to form (2). The removal of the hydrogen atom permits the dichlorocarbene to reach the reactive double bond.

syn-Oxabenzosesquinorbornene (1) was prepared by treatment of 2-norborneno[*c*]furan (7) with benzyne (8) generated from anthranilic acid (9). Adduct (10) was formed when an excess of benzyne was present (Combs, 1983). This is analogous to the reactions of isodicyclopentadiene (Paquette, Carr, Böhm & Gleiter, 1980); however, in the case of (7) a third crystalline product was obtained. The ^{13}C and ^1H NMR's of the unknown compound indicated the oxabenzosesquinorbornene framework was still present, but an asymmetric substitution had occurred at the reactive double bond. X-ray analysis showed the compound to be the adduct (3).



Experimental. All X-ray measurements made on a Syntex P_2 , diffractometer system, θ : 2θ scan, variable scan speed, graphite-monochromated radiation; lattice parameters by least-squares refinement of 15 medium-angle reflections measured by a centering routine

Table 1. *Atomic positional parameters ($\times 10^4$) and U_{eq} values ($\text{\AA}^2 \times 10^3$) for (1)*

	x	y	z	$U_{eq}\dagger$
C(1)	1591 (1)	4521 (3)	4588 (3)	41
C(2)	980 (1)	3342 (3)	4413 (3)	35
C(3)	606 (1)	4610 (3)	3375 (3)	37
C(4)	1015 (1)	6447 (3)	2952 (4)	45
C(4a)	1537 (1)	5691 (3)	1786 (4)	42
C(5)	1643 (1)	5087 (4)	-86 (4)	48
C(6)	1365 (1)	2921 (4)	-296 (4)	53
C(7)	1784 (1)	1538 (3)	856 (4)	48
C(8)	2260 (1)	3111 (4)	1622 (4)	44
C(8a)	1895 (1)	4508 (3)	2803 (4)	38
C(9)	2338 (1)	4516 (4)	24 (4)	54
O(10)	1349 (1)	6602 (2)	4598	52
C(11)	771 (1)	1481 (4)	5017 (4)	42
C(12)	166 (1)	918 (4)	4594 (4)	51
C(13)	-204 (1)	2159 (4)	3579 (4)	54
C(14)	13 (1)	4058 (4)	2933 (4)	46

$$\dagger U_{eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* (\mathbf{a}_i \cdot \mathbf{a}_j)$$

associated with the diffractometer system; intensities of equivalent reflections averaged; space groups determined from systematic absences; reference reflections showed no significant changes in intensities; Lorentz and polarization but no absorption corrections; direct methods (*MULTAN*78: Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) used to locate all heavy atoms, $\sum_w (|F_o| - |F_c|)^2$ minimized, $w = 1/\sigma^2(F_o)$, locally written programs used for data reduction, *MULTAN*78 for direct-methods' calculations and *XRAY*76 (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976) for all other computations; atomic scattering factors for C, N, O and Cl (including f') from Cromer & Mann (1968), those for H from Stewart, Davidson & Simpson (1965).

Compound (1). Crystal $0.5 \times 0.5 \times 0.5$ mm, 1129 independent reflections, $2\theta_{\max} = 54^\circ$ ($0 \leq h \leq 26$, $0 \leq k \leq 8$, $0 \leq l \leq 9$), 1026 with $I > 3\sigma(I)$, systematic absences $k+l=2n+1$ for $0kl$ and $h=2n+1$ for $h0l$, H atoms located in difference Fourier map, positional parameters for three H atoms refined, remaining H-atom parameters and all thermal parameters held fixed; full-matrix least-squares refinement gave $R = 0.046$, $R_w = 0.060$, $S = 4.06$ for 154 parameters, $(\Delta/\sigma)_{av} = 0.08$, $(\Delta/\sigma)_{\max} = 0.15$ (excluding H atoms), highest peak in final difference Fourier map $0.2 \text{ e } \text{\AA}^{-3}$; although Pna_2 is a polar space group, polar dispersion errors (Ueki, Zalkin & Templeton, 1966; Cruickshank & McDonald, 1967) were ignored due to the use of Mo $K\alpha$ radiation with only one O atom in the molecule. The atomic positional parameters are presented in Table 1 while selected distances are given in Table 4.

Compound (2). Poor-quality crystal, $0.5 \times 0.5 \times 0.15$ mm, 2318 independent reflections, $2\theta_{\max} = 51^\circ$ ($0 \leq h \leq 16$, $0 \leq k \leq 33$, $0 \leq l \leq 7$), 1795 with $I > 3\sigma(I)$, systematic absences $l=2n+1$ for $00l$, H-atom positions calculated, checked with difference map, not refined; full-matrix least-squares refinement gave $R = 0.060$, $R_w = 0.067$, $S = 2.69$ for 343 parameters, $(\Delta/\sigma)_{av} = 0.15$, $(\Delta/\sigma)_{\max} = 0.85$, highest peak in final

difference map $0.35 \text{ e } \text{\AA}^{-3}$. The atomic positional parameters are presented in Table 2 while selected distances are given in Table 4.

Compound (3). Crystal $0.5 \times 0.18 \times 0.25 \text{ mm}$, 2335 independent reflections, $2\theta_{\max} = 120^\circ$ ($0 \leq h \leq 12$, $0 \leq k \leq 19$, $-8 \leq l \leq 8$), 1897 with $I > 3\sigma(I)$, H atoms found in difference map and refined, thermal parameters held fixed; full-matrix least-squares refinement gave $R = 0.043$, $R_w = 0.053$, $S = 0.366$, 312 parameters refined, $(\Delta/\sigma)_{av} = 0.05$, $(\Delta/\sigma)_{\max} = 0.09$ (excluding H atoms), highest peak in final difference map $0.30 \text{ e } \text{\AA}^{-3}$. The atomic positional parameters are presented in Table 3 while selected distances are given in Table 4.[†]

Discussion. Compound (1). Fig. 1 is an ORTEP (Johnson, 1971) drawing of (1). The most significant feature of the structure is the $157.9(3)^\circ$ interplanar angle between $C(1)C(4)C(4a)C(8a)$ and $C(4a)C(5)-C(8)C(8a)$. This $22.1(3)^\circ$ deviation from planarity is significantly greater than the 16.4 to 18.0° bend observed for *syn*-sesquinorbornene *exo*-anhydride, 2-*exo*-(phenylsulfonyl)-*syn*-sesquinorbornene (Watson, Galloy, Bartlett & Roof, 1981), *syn*-oxasesquinorbornene *exo*-anhydride (Hagenbuch, Vogel, Pinkerton & Schwarzenbach, 1981), and two spiro derivatives (Paquette, Charumilind, Böhm, Gleiter, Bass & Clardy, 1983). The pyramidalization of the sp^2 carbon atoms has been attributed to asymmetric ground-state torsional interactions between the bridgehead hydrogen atoms, e.g. H(1), and the allylic bonds (Houk, 1983; Houk, Rondan, Brown, Jorgensen, Madura & Spellmeyer, 1983) or to antibonding hyperconjugative interactions between the π system and σ and σ^* orbitals (Gleiter & Böhm, 1983; Vogel, 1983; Spanget-Larsen & Gleiter, 1983). Whether the increased bending in (1) can be attributed to the effects described above cannot yet be ascertained. The $C(4a)-C(8a)$ distance is $1.339(3) \text{ \AA}$.

The interplanar angle between the phenyl ring and the $C(1)C(2)C(3)C(4)$ plane is $178.9(3)^\circ$. The significance of this 1.1° deviation from planarity is questionable; however, it is in the direction predicted by torsional and hyperconjugative interactions. The methylene and the oxa bridges are bent away from the *exo* π density of the central double bond. The most significant intramolecular contacts are $H(9ex)\cdots H(6ex)$ and $H(9ex)\cdots H(7ex)$ of 2.50 and 2.57 \AA . There are seven intermolecular contacts involving hydrogen atoms which range from 2.38 to 2.63 \AA .

Table 2. *Atomic positional parameters ($\times 10^4$) and U_{eq} values ($\text{\AA}^2 \times 10^3$) for (2)*

Molecule (I)	x	y	z	U_{eq}^\dagger
C(1)	6253 (5)	5086 (2)	6364 (11)	37
C(2)	6294 (4)	5567 (2)	7346 (11)	33
C(3)	5936 (5)	5886 (2)	5922 (10)	33
C(4)	5699 (5)	5568 (2)	4063 (10)	37
C(4a)	4845 (4)	5254 (2)	4468 (9)	30
C(5)	3797 (5)	5383 (3)	5237 (12)	45
C(6)	3936 (5)	5692 (2)	7181 (12)	43
C(7)	4329 (6)	5346 (3)	8801 (13)	51
C(8)	4410 (5)	4872 (3)	7642 (11)	44
C(8a)	5212 (5)	4905 (2)	6064 (10)	31
C(9)	3454 (5)	4941 (3)	6404 (14)	47
O(10)	6506 (4)	5253 (2)	4327 (8)	44
C(11)	6668 (4)	5731 (3)	9184 (11)	45
C(12)	6693 (5)	6226 (3)	9456 (12)	46
C(13)	6231 (6)	6530 (3)	8022 (15)	53
C(14)	5961 (5)	6375 (2)	6193 (11)	36
C(15)	4995 (6)	4730 (2)	3880 (11)	41
Cl(16)	4104 (2)	4309.7 (7)	3166 (4)	65
Cl(17)	5953 (2)	4539.9 (7)	2187 (4)	63
Molecule (II)				
C(1)	1082 (5)	2858 (3)	11220 (11)	39
C(2)	1085 (4)	2381 (3)	12131 (11)	38
C(3)	1501 (5)	2078 (2)	10610 (10)	34
C(4)	1691 (5)	2403 (3)	8845 (10)	38
C(4a)	2514 (4)	2756 (2)	9279 (10)	32
C(5)	3535 (4)	2651 (2)	10133 (11)	33
C(6)	3438 (4)	2330 (2)	12032 (12)	39
C(7)	2996 (4)	2673 (2)	13676 (9)	32
C(8)	2879 (4)	3140 (2)	12515 (10)	33
C(8a)	2077 (5)	3086 (2)	10899 (9)	30
C(9)	3834 (5)	3105 (2)	11263 (12)	42
O(10)	859 (3)	2704 (2)	9144 (8)	41
C(11)	698 (4)	2174 (3)	13890 (12)	37
C(12)	694 (6)	1692 (3)	14096 (13)	48
C(13)	1088 (6)	1392 (3)	12596 (15)	61
C(14)	1488 (5)	1583 (3)	10855 (13)	46
C(15)	2257 (5)	3282 (2)	8775 (10)	34
Cl(16)	3107 (2)	3721.8 (7)	8094 (4)	57
Cl(17)	1300 (2)	3439.3 (7)	7027 (3)	54

$\dagger U_{eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* (a_i \cdot a_j)$.

Compound (2). Fig. 2 is an ORTEP (Johnson, 1971) drawing of (2) while Fig. 3 shows important valence angles, interplanar angles and intramolecular contacts. The poor quality of the crystals led to molecular parameters of low accuracy, but the two independent molecules provide an internal check on important molecular features.

Compound (2) contains a number of short intramolecular contacts. The $Cl\cdots O$ distances of $2.567(6)$ and $2.568(6) \text{ \AA}$ are much shorter than the sum of acceptable van der Waals radii. The $H(9en)\cdots Cl$ distances for calculated hydrogen-atom positions are 2.09 and 2.14 \AA . The $Cl-C-Cl$ angle in similar compounds is around 109° (Wiberg, Burgmaier, Shen, LaPlaca, Hamilton & Newton, 1972), but the angles in (2) are compressed to $98.5(3)$ and $98.9(3)^\circ$. The separations between $H(9ex)$ and $H(6ex)$ and $H(7ex)$ range from 2.39 to 2.50 \AA , while $H(6en)\cdots C(3)$ is 2.25 and 2.28 \AA and $H(7en)\cdots C(2)$ is 2.21 and 2.27 \AA . It would appear that a reduction in the interplanar angle between $C(5)C(9)C(8)$ and $C(5)C(6)C(7)C(8)$ might release some strain; however, the $H(9ex)\cdots Cl$, $H(6en)\cdots C(3)$ and $H(7en)\cdots C(2)$ interactions appear to be attractive. The atoms $H(6en)$

[†] Lists of structure factors, anisotropic thermal parameters, hydrogen-atom parameters, interatomic distances, valence angles and interplanar angles have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39239 (56 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 3. Atomic positional parameters ($\times 10^4$) and U_{eq} values ($\text{\AA}^2 \times 10^3$) for (3)

	x	y	z	$U_{eq}\dagger$
C(1)	2737 (2)	5122 (1)	777 (3)	42 (2)
C(2)	2211 (2)	5851 (1)	606 (3)	36 (1)
C(3)	1144 (2)	5763 (1)	1226 (3)	39 (1)
C(4)	1055 (2)	4990 (1)	1734 (3)	41 (2)
C(4a)	1735 (2)	4793 (1)	3423 (3)	39 (1)
C(5)	1759 (2)	5179 (1)	5222 (4)	50 (2)
C(6)	1860 (2)	5987 (2)	5059 (4)	51 (2)
C(7)	3057 (2)	6094 (1)	4374 (4)	46 (2)
C(8)	3503 (2)	5333 (1)	4217 (4)	46 (2)
C(8a)	2943 (2)	4898 (1)	2729 (3)	38 (1)
C(9)	2943 (3)	4990 (2)	5830 (4)	58 (2)
O(10)	1781 (1)	4670 (1)	416 (2)	47 (1)
C(11)	2564 (2)	6492 (1)	-76 (4)	47 (2)
C(12)	1819 (2)	7051 (1)	-119 (4)	57 (2)
C(13)	754 (2)	6969 (2)	506 (4)	61 (2)
C(14)	399 (2)	6324 (1)	1185 (4)	52 (2)
C(15)	1578 (2)	3991 (1)	3718 (4)	48 (2)
O(15)	777 (1)	3670 (1)	4276 (3)	59 (1)
N(16)	2545 (2)	3678 (1)	3274 (3)	50 (1)
C(17)	3015 (2)	2991 (1)	3223 (3)	42 (2)
C(18)	2525 (2)	2336 (1)	3626 (4)	53 (2)
C(19)	3193 (3)	1740 (1)	3421 (4)	50 (2)
C(20)	4271 (3)	1809 (1)	2828 (4)	54 (2)
C(21)	4724 (2)	2460 (1)	2448 (4)	53 (2)
C(22)	4080 (2)	3058 (1)	2645 (3)	42 (2)
C(23)	4316 (2)	3827 (1)	2309 (3)	43 (2)
O(23)	5135 (1)	4138 (1)	1759 (2)	48 (1)
N(24)	3352 (2)	4152 (1)	2728 (3)	47 (1)

$\dagger U_{eq} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* (\mathbf{a}_i \cdot \mathbf{a}_j)$.

Table 4. Selected interatomic distances (\AA)

	(1)	(2)	(3)
	(I)	(II)	
C(1)—C(2)	1.530 (3)	1.50 (1)	1.47 (1)
C(1)—C(8a)	1.515 (4)	1.54 (1)	1.532 (9)
C(1)—O(10)	1.451 (3)	1.459 (9)	1.463 (9)
C(2)—C(3)	1.401 (3)	1.389 (9)	1.43 (1)
C(3)—C(4)	1.519 (3)	1.550 (9)	1.50 (1)
C(4)—C(4a)	1.518 (4)	1.499 (9)	1.539 (9)
C(4)—O(10)	1.454 (3)	1.436 (8)	1.444 (8)
C(4a)—C(5)	1.504 (4)	1.576 (9)	1.547 (9)
C(4a)—C(8a)	1.339 (3)	1.523 (9)	1.534 (9)
C(5)—C(6)	1.539 (4)	1.56 (1)	1.55 (1)
C(5)—C(9)	1.545 (3)	1.54 (1)	1.54 (1)
C(6)—C(7)	1.550 (4)	1.54 (1)	1.57 (1)
C(7)—C(8)	1.563 (3)	1.54 (1)	1.530 (9)
C(8)—C(8a)	1.504 (3)	1.52 (1)	1.541 (9)
C(8)—C(9)	1.536 (4)	1.56 (1)	1.559 (9)
C(4a)—C(15)	—	1.541 (9)	1.558 (9)
C(8a)—C(15), N(24)	—	1.54 (1)	1.52 (1)
C(15)—O(15)	—	—	—
C(15)—N(16)	—	—	—
N(16)—N(24)	—	—	—
C(23)—O(23)	—	—	—
C(23)—N(24)	—	—	—

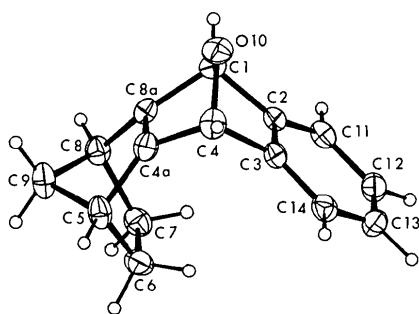


Fig. 1. ORTEP drawing of (1). Thermal ellipsoids are drawn at the 40% probability level.

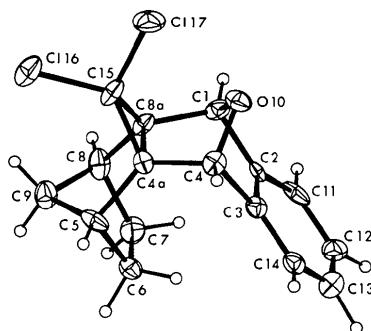


Fig. 2. ORTEP drawing of (2), a dichlorocarbene adduct of (1). Thermal ellipsoids are drawn at the 35% probability level.

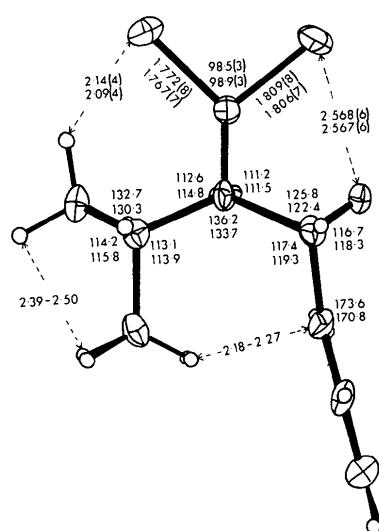


Fig. 3. Side of (2) showing important intramolecular distances (\AA), interplanar angles ($^\circ$, e.s.d. 0.6–0.9°) and valence angles ($^\circ$).

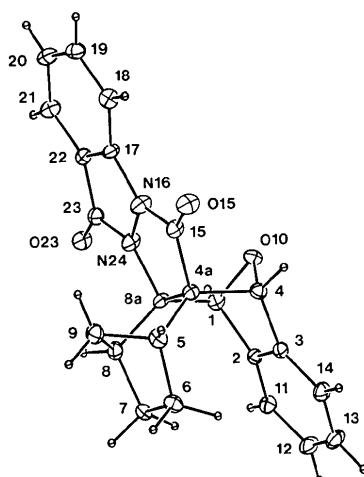


Fig. 4. ORTEP drawing of (3). Thermal ellipsoids are drawn at the 35% probability level.

and H(7en) lie within the π cloud of the carbon atoms C(2) and C(3). Normally, the interplanar angle between the phenyl ring and C(1)C(2)C(3)C(4) is expected to deviate from planarity by 1 to 4° with the phenyl ring bent in the *endo* direction. However, in (2) the deviation from planarity is 6.4 and 9.2° for the two independent molecules, and the bending is in the *exo* direction. The pyramidalization of the carbon atoms is consistent with an asymmetric π -electron density at C(2) and C(3) with the π -electron cloud attracted to the hydrogen atoms on the *endo* side.

Compound (3). Fig. 4 is an *ORTEP* drawing of (3). The *N*-formylindazolone moiety does not create as serious a steric problem as does dichlorocarbene. This is reflected in the relaxation of the interplanar angles and by an increase in intramolecular contact distances, e.g. angles between planes C(1)C(2)C(3)C(4) and the phenyl group, C(4a)C(5)C(8)C(8a) and C(5)-C(9)C(18), and C(5)C(6)C(7)C(8) and C(5)C(9)C(8) are 120.5 (4), 121.4 (4), and 118.1 (4) $^\circ$ in (3) but 132.7 (6), 114.2 (6), and 113.1 (6) $^\circ$ in (2). H(6)...C(3) is 2.55 Å in (3) but 2.23 Å in (2). The shortest intramolecular contacts in (3) are H(9b)...H(6a) = 2.46 Å and H(9b)...H(7b) = 2.47 Å which are the values observed for most sesquenorbornene derivatives (Watson, Galloy, Bartlett & Roof, 1981; Pinkerton, Schwarzenbach, Stibbard, Carrupt & Vogel, 1981; Hagenbuch, Vogel, Pinkerton & Schwarzenbach, 1981). There are six intermolecular contacts involving hydrogen atoms which range from 2.42 to 2.64 Å.

A least-squares plane fitted to C(4a)C(8a)-C(15)...N(24) shows a maximum deviation from planarity of 0.01 (1) Å. The interactions of O(10) and H(9a) with C(15), N(16) and N(24) stabilize the planar conformation of the *N*-formylindazolone moiety. An sp^3 hybridization of N(16) and N(24) would lead to stronger electrostatic interactions with the localized electron pairs. The extent of delocalization is reflected in the bond lengths C(15)-N(16) = 1.352 (3), N(16)-N(24) = 1.383 (3) and C(23)-N(24) = 1.354 (3) Å.

The C(2) and C(3) carbon atoms of the phenyl ring are pyramidalized and C(1)C(2)C(3)C(4) makes an interplanar angle of 176.6 (4) $^\circ$ with the phenyl ring. Like the dichlorocarbene adduct the phenyl ring is bent toward the O(10) face. The 3.4 (4) $^\circ$ bend is much smaller than the 6.4 (6) and 9.2° (6) $^\circ$ bends for the two independent molecules in the dichlorocarbene adduct. Although H(6b) and H(7b) lie directly above C(3) and C(2) as in the dichlorocarbene adduct, the H(6b)...C(3) and H(7b)...C(2) distances are about 0.3 Å longer. There is a weaker interaction between the two hydrogen atoms and the π cloud at C(2) and C(3), and the degree of pyramidalization of the two carbon atoms is reduced.

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