Table 2. *Experimental values of angles in the benzene ring and the difference between these and the values obtained from the Domenicano & Murray-Rust rules (Δ, in degrees)*

2,5-Dinitrobenzoic acid		2,4-Dinitrobenzoic acid		*o*-Nitrobenzoic acid	
Angle	Δ	Angle	Δ	Angle	Δ
117·4	−1·1	117·9	−0·7	116·2	−2·0
122·7	−0·4	122·9	−0·1	123·7	0·0
119·0	0·5	116·6	0·3	118·4	0·2
118·8	0·2	123·4	0·0	120·6	0·1
122·5	−0·9	118·2	−0·4	119·8	−0·7
119·5	1·3	120·9	0·5	121·2	1·1

distinctly deformed in comparison with the values expected by the additive influence of substituents.

The benzene ring and carboxyl group are nearly coplanar for 2,5-DNBA, the angle between the planes being 4·0°. The NO_2 substituent in the *ortho* position is nearly perpendicular to the benzene ring, with interplanar angle 86·0°. The angle between the planes of the carboxy and nitro groups in the *ortho* position is 89·8°. A similar finding is observed for 2,4-DNBA (Więckowski & Krygowski, 1985), the angle between neighbouring NO_2 and COOH substituents being 64·4°. For *o*-nitrobenzoic acid the carboxy and nitro groups make angles of 24·1° and 54·3°, respectively, with the aromatic plane (Tavale & Pant, 1973), and consequently the angle between COOH and NO_2 planes is 78·4°. On comparison of the above-mentioned structures we can say that neighbouring NO_2 and COOH groups are twisted by an angle of 60–90°.

The planes of the benzene ring and of the other nitro group are nearly coplanar. The angles found are: for *p*-nitrobenzoic acid 13·7° (Colapietro & Domenicano, 1977), 2,5-DNBA 14·3°, 2,4-DNBA 4·1° (Więckowski & Krygowski, 1985), *m*-nitrobenzoic acid 2·7 and 1·3° for *A* and *B* forms (Dhaneshwar, Kulkarni, Tavale & Pant, 1975). These results are in line with the conclusions of Holden & Dickinson (1977).

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Bicyclo[2.2.1]hepta-2,5-diene-2,3-dicarboxylic Anhydride (1), $C_9H_6O_3$, and Bicyclo[2.2.1]hept-2-ene-2,3-dicarboxylic Anhydride (2), $C_9H_8O_3$

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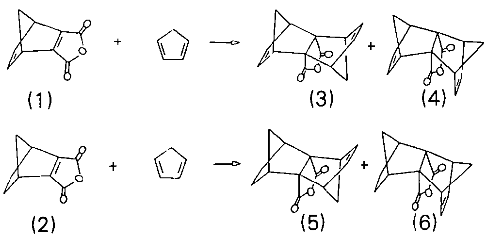
Abstract. (1) M_r = 162·15, monoclinic, $P2_1/n$, a = 12·642 (3), b = 11·412 (2), c = 11·773 (2) Å, β = 117·77 (2)°, V = 1502·9 (6) Å^3, Z = 8, D_x = 1·433 g cm^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, μ = 9·30 cm^{-1}, $F(000)$ = 672, T = 298 K, R = 0·046 for 1498 independent observed reflections. (2) M_r = 164·16, orthorhombic, *Pnma*, a = 6·233 (2), b = 10·421 (4), c = 11·843 (4) Å, V = 769·3 (5) Å^3, Z = 4, D_x =

1·417 g cm^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, μ = 9·09 cm^{-1}, $F(000) = 344$, $T = 298$ K, $R = 0{\cdot}049$ for 435 independent observed reflections. The anhydride ring and the associated carbonyl O atoms are coplanar in compounds (1) and (2). The C(2) and C(3) atoms are pyramidalized and the π-electron system in (2) deviates from planarity by 10·6 (6)° while the deviations for the two independent molecules in (1) are 1·9 (7) and 4·1 (7)°. The greater pyramidalization in the 8,9,10-trinorborn-2-ene anhydride (2) is consistent with theoretical predictions.

Introduction. Edman & Simmons (1968) found the addition of cyclopentadiene to 8,9,10-trinorborna-2,5-diene-2,3-dicarboxylic anhydride (1) gave a 60–70 to 1 ratio of cycloadducts (3) and (4). Adduct (3) is formed by addition to the *exo* face in an anti-Alder's-rule fashion (Alder, Pascher & Vogt, 1942) while (4) is formed by addition to the *exo* face according to Alder's rule. When cycloaddition is carried out with 8,9,10-trinorborn-2-ene-2,3-dicarboxylic anhydride (2), a significant yield of the *syn*-anhydride (6) is obtained (Bartlett, Blakeney, Kimura & Watson, 1980). The ratio of (5) to (6) is about 3:1 depending upon the reaction conditions. The reasons for the 20–40 fold difference in the geometry of addition are of practical and theoretical interest. A calculation by Wipff & Morokuma (1980) indicated the π-system of 8,9,10-trinorborn-2-ene deviated from planarity by 4·9° while that of 8,9,10-trinorborna-2,5-diene deviated by only 2·3°. The substituents at the 2,3-position are always bent away from the *exo* face, the side with the methylene bridge. A survey of the X-ray data for a number of compounds containing the 8,9,10-trinorborn-2-ene moiety showed that deviations from planarity of the order of 3 to 10° are a common feature (Watson, Galloy, Bartlett & Roof, 1981). Pyramidalization of the C(sp^2) atoms in 8,9,10-trinorborn-2-ene systems has been the subject of many recent theoretical and experimental papers (Watson, 1983; Houk, Rondan, Brown, Jorgensen, Madura & Spellmeyer, 1983; Spanget-Larsen & Gleiter, 1983; Paquette, Hsu, Gallucci, Korp, Bernal, Dravetz & Hathaway, 1984; Vogel, 1984; Pinkerton, Schwarzenbach, Birbaum, Carrupt, Schwager & Vogel, 1984).



Because of the large differences in stereochemical behavior of the anhydrides (1) and (2) upon the addition of cyclopentadiene, it was of interest to investigate in detail the structures of the two molecules.

Experimental. Syntex $P2_1$ diffractometer, θ:2θ scan, variable scan rate, $2\theta_{\max} = 120°$, graphite-monochromated Cu $K\alpha$ radiation; lattice parameters from least-squares refinement of 15 medium-angle reflections ($14{\cdot}04 \leq 2\theta \leq 27°$ for 1 and $11{\cdot}31 \leq 2\theta \leq 22{\cdot}73°$ for 2) with angles measured by a centering routine associated with the diffractometer system; Lorentz and polarization corrections; scans of several equivalent reflections showed variations in intensities for (2) to be of the same order as the check reflection while variations for (1) exceeded the check reflection but were within 3σ of the mean; no absorption correction applied; direct methods (*MULTAN*78: Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978); full-matrix least-squares refinement, $\sum w(|F_o| - |F_c|)^2$ minimized, $w = 1/\sigma^2(F_o)$ (derived from counting statistics).

(1) Crystal dimensions 0·58 × 0·35 × 0·28 mm, systematic absences $h + l = 2n+1$ for $h0l$ and $k = 2n+1$ for $0k0$ consistent with space group $P2_1/n$, $2/m$ Laue symmetry; monitored reflection 040 showed no significant change in intensity; 2054 independent reflections ($0 \leq h \leq 13$, $0 \leq k \leq 12$, $-12 \leq l \leq 11$), 1498 with intensities greater than $3\sigma(I)$; extinction corrections applied ($G = 8{\cdot}41$; Larson, 1967); H atoms located in difference Fourier map and positions constrained during refinement; H-atom positions scaled to a distance of 1·08 Å following refinement; $R = 0{\cdot}046$, $wR = 0{\cdot}053$, 218 parameters refined, $(\Delta/\sigma)_{\rm av} = 0{\cdot}12$, $(\Delta/\sigma)_{\max} = 0{\cdot}70$ (thermal parameter), $S = 2{\cdot}32$, 0·22 e Å^{-3} largest peak in final difference Fourier map.

(2) Crystal dimensions 0·55 × 0·42 × 0·33 mm, systematic absences $l = 2n+1$ for $0kl$ and $h = 2n+1$ for $hk0$ consistent with space groups *Pnma* and $Pna2_1$, refined parameters more acceptable for *Pnma*, *mmm* Laue symmetry; monitored reflection 121 showed no significant change in intensity; 561 independent reflections ($0 \leq h \leq 6$, $0 \leq k \leq 11$, $0 \leq l \leq 12$), 435 with intensities greater than $3\sigma(I)$, extinction corrections applied ($G = 2{\cdot}59$); H-atom positional parameters refined but thermal parameters fixed; H-atom positions scaled to 1·08 Å following refinement; $R = 0{\cdot}049$, $wR = 0{\cdot}070$, 72 parameters refined, $(\Delta/\sigma)_{\rm av} = 0{\cdot}01$, $(\Delta/\sigma)_{\max} = 0{\cdot}04$, $S = 3{\cdot}46$, 0·12 e Å^{-3} largest peak in final difference Fourier map.

Locally written program used for data reduction, *MULTAN*78 for direct-methods calculations, and *XRAY*76 (Stewart, Machin, Dickinson, Ammon, Heck & Flack, 1976) for all others; atomic scattering factors for C and O from Cromer & Mann (1968), for H from Stewart, Davidson & Simpson (1965), anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974). Tables 1 and 2 list atomic positions for compounds (1) and (2) while Table 3 lists interatomic distances, valence angles, and torsion angles.*

Discussion. Figs. 1 and 2 are *ORTEP* (Johnson, 1971) drawings of compounds (1) and (2). A comparison of interatomic distances and angles with the two independent molecules of (1) and with molecule (2) shows internal consistency. The most significant differences between molecules (1) and (2) involve the pyramidalization of the C(2) and C(3) atoms and the methylene-bridge interplanar angles. The

Table 1. *Fractional atom coordinates* (×10^4) *and* U_{eq} (Å^2 ×10^3) *values for compound* (1)

	x	*y*	*z*	$U_{\rm eq}$†
Molecule 1				
C(1)	5390 (3)	266 (3)	2292 (3)	63 (2)
C(2)	4817 (3)	1440 (3)	1739 (3)	56 (2)
C(3)	4510 (3)	1936 (3)	2548 (3)	55 (2)
C(4)	4841 (3)	1109 (3)	3675 (3)	64 (2)
C(5)	4064 (3)	20 (3)	3098 (3)	67 (2)
C(6)	4382 (3)	−461 (3)	2303 (3)	69 (2)
C(7)	6009 (3)	631 (3)	3719 (3)	73 (2)
C(8)	4405 (3)	2154 (3)	589 (3)	77 (2)
O(8)	4450 (3)	2019 (3)	−398 (2)	112 (2)
C(9)	3928 (3)	3052 (3)	2028 (4)	74 (2)
O(9)	3561 (2)	3815 (2)	2437 (3)	107 (2)
O(10)	3884 (2)	3151 (2)	811 (3)	89 (2)
Molecule 2				
C(1)	3669 (3)	3923 (3)	−4201 (3)	71 (2)
C(2)	4914 (3)	3743 (3)	−3090 (3)	55 (2)
C(3)	4859 (2)	3961 (2)	−2017 (3)	49 (2)
C(4)	3591 (3)	4289 (3)	−2355 (3)	58 (2)
C(5)	3332 (3)	5440 (3)	−3109 (3)	66 (2)
C(6)	3393 (3)	5225 (3)	−4166 (3)	79 (2)
C(7)	2969 (3)	3439 (3)	−3510 (3)	73 (2)
C(8)	6138 (3)	3457 (3)	−2788 (3)	66 (2)
O(8)	6594 (2)	3196 (2)	−3435 (2)	90 (2)
C(9)	6047 (3)	3842 (3)	−934 (3)	60 (2)
O(9)	6434 (2)	3967 (2)	192 (2)	83 (1)
O(10)	6808 (2)	3506 (2)	−1449 (2)	69 (1)

† $U_{\rm eq} = \frac{1}{3}[U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aba^*b^*\cos\gamma + 2U_{13}aca^*c^*\cos\beta + 2U_{23}bcb^*c^*\cos\alpha]$.

Table 2. *Fractional atomic coordinates* (×10^4) *and* U_{eq} (Å^2 ×10^3) *values for compound* (2)

	x	*y*	*z*	$U_{\rm eq}$‡
C(1)	2652 (6)	3588 (3)	4565 (3)	71 (2)
C(2)	3345 (5)	3139 (3)	5708 (2)	67 (2)
C(6)	244 (6)	3232 (3)	4507 (3)	71 (2)
C(7)	3595 (9)	2500†	3848 (4)	82 (3)
C(8)	3616 (5)	3595 (6)	6859 (3)	94 (3)
O(8)	3673 (4)	4648 (4)	7257 (3)	137 (3)
O(10)	3865 (6)	2500†	7535 (3)	113 (3)

† Restricted by space group.

‡ $U_{\rm eq} = \frac{1}{3}[U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aba^*b^*\cos\gamma + 2U_{13}aca^*c^*\cos\beta + 2U_{23}bcb^*c^*\cos\alpha]$.

Table 3. *Interatomic distances* (Å), *valence angles* (°) *and torsion angles* (°)

	Compound (1)		Compound (2)
	Molecule *A*	Molecule *B*	
C(1)—C(2)	1·518 (5)	1·521 (4)	1·496 (4)
C(1)—C(6)	1·526 (6)	1·531 (5)	1·547 (5)
C(1)—C(7)	1·544 (5)	1·556 (6)	1·534 (5)
C(2)—C(3)	1·313 (6)	1·321 (6)	1·332 (4)
C(2)—C(8)	1·453 (5)	1·454 (5)	1·454 (5)
C(3)—C(4)	1·520 (5)	1·508 (5)	—*
C(3)—C(9)	1·456 (5)	1·454 (4)	—
C(4)—C(5)	1·533 (5)	1·533 (5)	—
C(4)—C(7)	1·552 (6)	1·553 (4)	—
C(5)—C(6)	1·300 (6)	1·305 (6)	1·527 (5)
C(8)—O(8)	1·200 (5)	1·188 (5)	1·195 (7)
C(8)—O(10)	1·399 (5)	1·401 (4)	1·403 (6)
C(9)—O(9)	1·189 (5)	1·189 (4)	
C(9)—O(10)	1·412 (6)	1·408 (5)	
C(2)C(1)C(6)	104·5 (3)	105·4 (2)	104·2 (3)
C(2)C(1)C(7)	97·3 (3)	96·6 (3)	99·1 (3)
C(6)C(1)C(7)	98·0 (3)	97·9 (3)	99·8 (3)
C(1)C(2)C(3)	108·2 (3)	107·6 (3)	108·2 (3)
C(1)C(2)C(8)	141·9 (4)	142·9 (4)	141·2 (3)
C(3)C(2)C(8)	109·6 (3)	109·4 (2)	109·1 (3)
C(2)C(3)C(4)	108·2 (3)	108·5 (3)	—
C(2)C(3)C(9)	109·5 (3)	109·1 (3)	—
C(4)C(3)C(9)	142·2 (4)	142·3 (3)	—
C(3)C(4)C(5)	104·9 (2)	106·2 (3)	—
C(3)C(4)C(7)	96·8 (3)	96·8 (3)	—
C(5)C(4)C(7)	97·6 (3)	98·3 (2)	—
C(4)C(5)C(6)	108·2 (4)	107·4 (3)	—
C(1)C(6)C(5)	108·4 (3)	108·9 (3)	103·9 (3)
C(1)C(7)C(4)	93·8 (2)	93·3 (3)	95·4 (3)
C(2)C(8)O(8)	132·3 (4)	132·7 (3)	132·4 (4)
C(2)C(8)O(10)	106·1 (3)	106·4 (3)	106·4 (4)
O(8)C(8)O(10)	121·6 (3)	120·8 (3)	121·2 (3)
C(3)C(9)O(9)	133·4 (4)	133·4 (4)	—
C(3)C(9)O(10)	105·7 (3)	106·4 (3)	—
O(9)C(9)O(10)	120·9 (3)	120·3 (3)	—
C(8)O(10)C(9)	109·0 (3)	108·6 (2)	108·9 (3)
C(1)C(2)C(3)C(4)	−1·0 (4)	0·2 (3)	—
C(2)C(3)C(4)C(5)	−63·7 (4)	−64·7 (3)	—
C(3)C(4)C(5)C(6)	64·5 (4)	63·7 (3)	—
C(4)C(5)C(6)C(1)	0·0 (4)	1·1 (4)	—
C(5)C(6)C(1)C(2)	−65·0 (3)	−65·2 (4)	−66·7 (3)
C(6)C(1)C(2)C(3)	65·6 (3)	64·0 (4)	69·9 (3)
C(2)C(3)C(4)C(7)	36·1 (3)	36·0 (3)	32·7 (4)
C(3)C(4)C(7)C(1)	−53·9 (3)	−54·6 (3)	—
C(4)C(7)C(1)C(2)	53·4 (3)	54·4 (3)	49·7 (3)
C(7)C(1)C(2)C(3)	−34·7 (4)	−36·2 (3)	—
C(5)C(6)C(1)C(7)	34·8 (3)	34·0 (3)	35·4 (3)
C(6)C(1)C(7)C(4)	−52·4 (3)	−52·0 (2)	−56·6 (3)
C(1)C(7)C(4)C(5)	52·3 (3)	53·0 (3)	—
C(7)C(4)C(5)C(6)	−34·7 (3)	−35·9 (4)	—
C(8)C(2)C(3)C(9)	−3·1 (4)	0·4 (4)	—
C(2)C(3)C(9)O(10)	1·9 (4)	−1·5 (3)	−2·4 (4)
C(3)C(9)O(10)C(8)	0·1 (3)	1·9 (3)	—
C(9)O(10)C(8)C(2)	−1·9 (3)	−1·7 (4)	−3·8 (4)
O(10)C(8)C(2)C(3)	3·2 (4)	0·8 (4)	—

* Symmetry-related distances and angles.

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* Lists of structure factors, H-atom parameters and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42200 (28 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

pyramidalization results in a deviation of the π-system from planarity. The angle between the C(1)C(2)-C(3)C(4) and C(8)C(2)C(3)C(9) planes is 10·6 (6)° in (2) and 4·1 (7) and 1·9 (7)° in (1). This is consistent with other experimenal observations and with theoretical predictions. In addition to the anhydride moiety in (2) being bent away from the *exo* side of the molecule (methylene-bridge side), the angle between the C(1)C(7)C(4) and C(1)C(2)C(3)C(4) planes is 127·6 (5)° in (2) and 122·7 (5) and 121·6 (5)° in (1). These factors can be used to rationalize the differences in the cycloaddition-product distribution in the reaction of 8,9,10-trinorborn-2-ene and 8,9,10-trinorborna-2,5-diene anhydrides. In both compounds the pentadiene moiety approaches from the least-hindered *exo* face. This face has a slight excess of π-electron density due to the pyramidalization of the C(2) and C(3) atoms. Addition, according to Alder's rule, requires the methylene end of the pentadiene molecule to be oriented toward the methylene bridge. Anti-Alder's-rule addition occurs with the ethylene end of the cyclopentadiene oriented toward the methylene bridge. Because of the differences in pyramidalization in compound (2) with the associated folding of the π-system and the increased interplanar angle involving the methylene bridge, an Alder's-rule approach encounters less steric hindrance than in (1).

In 8,9,10-trinorborn-5-ene-2,3-*endo*-dicarboxylic anhydride (Destro, Filippini, Gramaccioli & Simonetta, 1969) the C(5) and C(6) atoms are pyramidalized with an 8·5° deviation of the π-system from planarity. In 8,9,10-trinorborn-5-ene-2,3-*exo*-dicarboxylic anhydride (Filippini, Gramaccioli, Rovere & Simonetta, 1972) the π-system is *assumed* to be planar and the H-atom positions are calculated. Such assumptions are probably invalid in many compounds with an unsymmetric double-bond environment. In compound (1) the C(5),C(6) π-systems deviate by 3 (1) and 6 (1)°. In general, the deviations in 8,9,10-trinorborna-2,5-dienes are smaller than in 8,9,10-trinorbornenes, but inaccuracies in H-atom positions prohibit accurate comparisons.

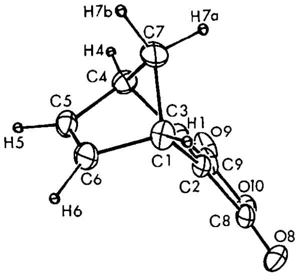

Fig. 1. *ORTEP* drawing of compound (1). Thermal ellipsoids are drawn at the 55% probability level.

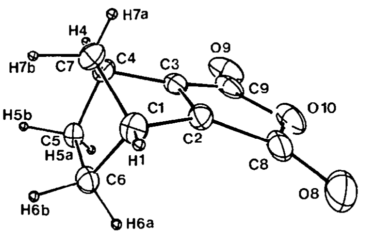

Fig. 2. *ORTEP* drawing of compound (2). Thermal ellipsoids are drawn at the 55% probability level.

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