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***rel*-(1*R*,4*S*,4a*R*,7*R*)- (1) and *rel*-(1*R*,4*S*,4a*S*,7*S*)- (2) Isomers of 1,2,3,4,4a,5,6,7-Octahydro-1,4:4a,7-dimethanonaphthalene-5,5,6,6-tetracarbonitrile, $C_{16}H_{12}N_4$**

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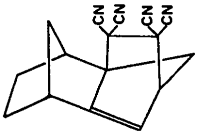
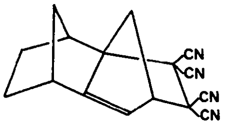
Abstract. Compound (1): $M_r = 260{\cdot}30$, monoclinic, $P2_1/c$, $a = 8{\cdot}986\,(3)$, $b = 9{\cdot}661\,(3)$, $c = 14{\cdot}870\,(4)$ Å, $\beta = 94{\cdot}86\,(2)°$, $V = 1286{\cdot}3\,(7)$ Å^3, $Z = 4$, $D_x = 1{\cdot}344$ g cm^{-3}, Cu $K\alpha$, $\lambda = 1{\cdot}54178$ Å, $\mu = 6{\cdot}77$ cm^{-1}, $F(000) = 544$, room temperature, $R = 0{\cdot}0397$ for 1494 unique reflections with $I > 3\sigma(I)$. Compound (2): $M_r = 260{\cdot}30$, monoclinic, $P2_1/c$, $a = 9{\cdot}696\,(2)$, $b = 8{\cdot}925\,(1)$, $c = 16{\cdot}022\,(4)$ Å, $\beta = 105{\cdot}33\,(2)°$, $V = 1337{\cdot}1\,(5)$ Å^3, $Z = 4$, $D_x = 1{\cdot}293$ Mg m^{-3}, Cu $K\alpha$, $\lambda = 1{\cdot}54178$ Å, $\mu = 6{\cdot}51$ cm^{-1}, $F(000) = 544$, room temperature, $R = 0{\cdot}0345$ for 1447 unique reflections, $I > 3\sigma(I)$. The molecules are composed of end-to-edge fused norbornane systems. The sixteen C(sp^3) valence angles of less than 105° imply considerable ring strain. C—C bond lengths of 1·577 (3) to 1·620 (3) Å are associated with the tetracyanoethylene moiety. The bond elongation is attributed to the electron-withdrawing character of the cyano groups.



(1)



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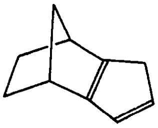
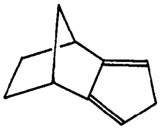


(3)



(4)

Introduction. At elevated temperatures (3) is in equilibrium with isodicyclopentadiene (4) (Bartlett & Wu, 1983). Isomer (3) is more reactive and will preferentially form cycloadducts (Subramanyan, Bartlett, Iglesias, Watson & Galloy, 1982; Paquette, Williams, Carr, Charumilind & Blount, 1982). When isodicyclopentadiene (4) is added to a refluxing solution of tetracyanoethylene (TCNE) in *m*-dichlorobenzene, the thermally stable products (1) and (2) are formed in a 3:1 ratio. Spectral data were consistent with a [6.2.1.1^{2,5}.0^{1,6}]dodec-6(7)-ene system which is confirmed by the present study. No cycloadducts of TCNE with (4) were found. Cycloadducts of TCNE with (4) are formed at lower temperatures; however, they undergo *retro*-Diels–Alder reactions even at room temperature. Adducts (1) and (2) can also be prepared by heating the adducts of (4) in *m*-dichlorobenzene at 423 K for 30 min (Bartlett & Wu, 1984).

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,

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angles measured by centering routine associated with the diffractometer system; systematic absences $l = 2n+1$ for $h0l$ and $k = 2n+1$ for $0k0$; monitored reflections showed no significant changes in intensity; Lorentz and polarization, no absorption corrections; direct methods (*MULTAN*78: Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) used to locate heavy atoms, hydrogen-atom positions from difference map; full-matrix least-squares anisotropic refinement (H atoms not refined), $\sum w(|F_o| - |F_c|)^2$ minimized, $w = 1/\sigma^2(F_o)$; locally written programs used for data reduction and initial block-diagonal least-squares refinement, *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, O and N from Cromer & Mann (1968), for H from Stewart, Davidson & Simpson (1965).

Compound (1). Prismatic-shaped crystal, 0·33 × 0·27 × 0·22 mm, 1755 independent reflections ($0 \le h \le 9$, $0 \le k \le 10$, $-15 \le l \le 15$), 1494 with $I > 3\sigma(I)$, $R = 0{\cdot}0397$, $R_w = 0{\cdot}052$, $S = 2{\cdot}58$, $(\Delta/\sigma)_{av} = 0{\cdot}02$, $(\Delta/\sigma)_{max} = 0{\cdot}14$, largest peak in final difference map 0·25 e Å^{-3}. Table 1 lists atomic positional parameters.

Compound (2). Needle-shaped crystal, 0·50 × 0·23 × 0·18 mm, 1826 independent reflections ($0 \le h \le 10$, $0 \le k \le 9$, $-16 \le l \le 16$), 1447 with $I > 3\sigma(I)$, $R = 0{\cdot}0345$, $R_w = 0{\cdot}044$, $S = 2{\cdot}06$, $(\Delta/\sigma)_{av} = 0{\cdot}015$, $(\Delta/\sigma)_{max} = 0{\cdot}10$, largest peak in the final difference map 0·13 e Å^{-3}. Table 2 lists atomic positional parameters.*

Table 1. *Fractional atomic coordinates* (×10^4) *and equivalent isotropic thermal parameters* (Å^2 ×10^3) *for compound* (1)

	x	y	z	U_{eq}*
C(1)	2825 (2)	1141 (2)	8896 (1)	39 (1)
C(2)	3523 (2)	2666 (2)	8845 (1)	36 (1)
C(3)	2836 (2)	3423 (2)	9683 (1)	36 (1)
C(4)	1859 (2)	2223 (2)	10046 (1)	43 (1)
C(5)	578 (2)	1935 (2)	9343 (2)	45 (1)
C(6)	1158 (2)	1276 (2)	8679 (1)	39 (1)
C(7)	754 (2)	385 (2)	7863 (1)	48 (1)
C(8)	883 (3)	−1106 (3)	8231 (2)	59 (2)
C(9)	2570 (3)	−1317 (3)	8451 (2)	59 (2)
C(10)	3261 (2)	69 (2)	8197 (2)	50 (1)
C(11)	2185 (3)	469 (2)	7386 (2)	52 (1)
C(12)	2881 (2)	989 (2)	9931 (1)	45 (1)
C(13)	3157 (2)	3433 (2)	7999 (1)	39 (1)
N(13)	2899 (2)	4030 (2)	7343 (1)	57 (1)
C(14)	5171 (2)	2552 (2)	8970 (1)	40 (1)
N(14)	6424 (2)	2411 (2)	9056 (1)	58 (1)
C(15)	1939 (2)	4656 (2)	9433 (1)	42 (1)
N(15)	1196 (2)	5589 (2)	9264 (1)	61 (1)
C(16)	4008 (2)	3808 (2)	10397 (1)	40 (1)
N(16)	4869 (2)	4075 (2)	10973 (1)	55 (1)

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

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

U_{eq} is defined in Table 1.

	x	y	z	U_{eq}(Å^2)
C(1)	7387 (2)	7476 (2)	6654 (1)	40 (1)
C(2)	7641 (2)	8366 (2)	5840 (1)	40 (1)
C(3)	9090 (2)	7583 (2)	5730 (1)	44 (1)
C(4)	9396 (2)	6405 (2)	6491 (1)	48 (1)
C(5)	8237 (2)	5222 (2)	6281 (1)	51 (1)
C(6)	7055 (2)	5856 (2)	6380 (1)	44 (1)
C(7)	5654 (3)	5486 (2)	6561 (1)	57 (1)
C(8)	4445 (2)	6422 (3)	5985 (2)	62 (1)
C(9)	4758 (3)	8039 (2)	6337 (1)	59 (1)
C(10)	6162 (2)	7876 (2)	7054 (1)	51 (1)
C(11)	5910 (3)	6350 (3)	7428 (1)	63 (1)
C(12)	8949 (2)	7320 (2)	7189 (1)	49 (1)
C(13)	6502 (2)	8211 (2)	5037 (1)	44 (1)
N(13)	5650 (2)	8065 (2)	4397 (1)	66 (1)
C(14)	7848 (2)	9973 (2)	6059 (2)	53 (1)
N(14)	8021 (2)	11188 (2)	6267 (2)	85 (1)
C(15)	10274 (2)	8660 (3)	5845 (1)	55 (1)
N(15)	11203 (2)	9481 (3)	5943 (2)	82 (1)
C(16)	8896 (2)	6856 (2)	4883 (2)	50 (1)
N(16)	8761 (2)	6257 (2)	4238 (1)	69 (1)

Discussion. Fig. 1 and 2 are *ORTEP* drawings (Johnson, 1971) of compounds (1) and (2). In general, there is good agreement of equivalent bond lengths between the two isomers; however, there are differences in intramolecular interactions. In (1) H(9*a*) and H(12*a*) are separated by 2·29 (4) Å on the *endo* side of the molecule while in (2) H(11*a*) and H(12*b*) are separated by 2·36 (4) Å on the *exo* side. The short interaction in (1) may be responsible for the significant difference in the C(10)C(1)C(12) valence angle between (1) (128·3°) and (2) (123·1°). It might be expected that these interactions should lead to interplanar angle *A–C* (see Table 3) being larger in (2) and *A–B* being larger in (1); however, the opposite trend is observed; *A–C* and *A–B* are 126·0 (6) and 110·5 (6)° in (1) and 121·4 (6) and 115·5 (6)° in (2). The values of the *B–C* interplanar angles of 123·1 (6) and 123·6 (6)° are constant in most norbornane derivatives (Watson, Galloy, Bartlett & Roof, 1981; Pinkerton, Schwarzenbach, Stibbard, Carrupt & Vogel, 1981). The interplanar angle is determined primarily by the H(11*b*)···H(8*b*) and H(11*b*)···H(9*b*) separations which range from 2·41 (4) to 2·56 (4) Å.

The separation between the π systems, *e.g.* C(6)···C(13), of 2·883 (3) and 2·987 (3) Å may indicate some π-electron interaction. C(13) also lies within 2·53 (4) Å of H(11*a*) in (1) and 2·54 (4) Å of H(9*a*) in (2). The N—C—C—C—N units are planar within each molecule. The units adjacent to the C(11) bridge make interplanar angles of 93·9 (5) and 94·0 (5)° with C(1)C(2)C(3)-C(4) while the other N—C—C—C—N units make interplanar angles of 90·6 (5) and 90·1 (5)°. The two

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* Lists of structure factors, hydrogen-atom coordinates and thermal parameters for (1) and (2) have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39151 (34 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

	Compound (1)	Compound (2)		Compound (1)	Compound (2)
C(1)–C(2)	1·606 (3)	1·601 (3)	C(5)–C(6)	1·319 (3)	1·325 (3)
C(1)–C(6)	1·511 (3)	1·521 (3)	C(6)–C(7)	1·507 (2)	1·499 (4)
C(1)–C(10)	1·541 (3)	1·533 (3)	C(7)–C(8)	1·542 (4)	1·534 (3)
C(1)–C(12)	1·543 (2)	1·537 (2)	C(7)–C(11)	1·522 (3)	1·550 (3)
C(2)–C(3)	1·612 (2)	1·620 (3)	C(8)–C(9)	1·537 (4)	1·550 (4)
C(2)–C(13)	1·473 (2)	1·464 (2)	C(9)–C(10)	1·537 (4)	1·539 (3)
C(2)–C(14)	1·481 (3)	1·478 (3)	C(10)–C(11)	1·530 (4)	1·533 (3)
C(3)–C(4)	1·577 (3)	1·578 (2)	C(13)–N(13)	1·140 (2)	1·141 (2)
C(3)–C(15)	1·468 (3)	1·471 (3)	C(14)–N(14)	1·131 (3)	1·134 (3)
C(3)–C(16)	1·478 (2)	1·471 (3)	C(15)–N(15)	1·137 (3)	1·139 (3)
C(4)–C(5)	1·514 (3)	1·514 (3)	C(16)–N(16)	1·134 (2)	1·140 (3)
C(4)–C(12)	1·523 (3)	1·537 (3)			
C(2)C(1)C(6)	107·2 (1)	107·6 (1)	C(5)C(4)C(12)	102·1 (1)	101·4 (2)
C(2)C(1)C(10)	117·5 (1)	121·9 (1)	C(4)C(5)C(6)	106·3 (2)	106·9 (2)
C(2)C(1)C(12)	98·9 (1)	99·1 (1)	C(1)C(6)C(5)	109·2 (1)	108·5 (2)
C(6)C(1)C(10)	102·6 (1)	102·3 (2)	C(1)C(6)C(7)	106·8 (1)	106·7 (2)
C(6)C(1)C(12)	99·7 (1)	100·2 (1)	C(5)C(6)C(7)	142·7 (2)	141·8 (2)
C(10)C(1)C(12)	128·3 (2)	123·1 (1)	C(6)C(7)C(8)	104·0 (2)	110·6 (2)
C(1)C(2)C(3)	101·7 (1)	101·5 (1)	C(6)C(7)C(11)	100·9 (2)	97·2 (2)
C(1)C(2)C(13)	116·2 (1)	115·2 (2)	C(8)C(7)C(11)	100·0 (2)	100·6 (2)
C(1)C(2)C(14)	108·4 (2)	109·2 (2)	C(7)C(8)C(9)	104·0 (2)	104·1 (2)
C(3)C(2)C(13)	111·1 (1)	109·8 (1)	C(8)C(9)C(10)	104·1 (2)	103·5 (2)
C(3)C(2)C(14)	112·4 (1)	112·2 (2)	C(1)C(10)C(9)	106·8 (2)	109·9 (2)
C(13)C(2)C(14)	107·0 (1)	108·9 (2)	C(1)C(10)C(11)	100·5 (2)	100·2 (2)
C(2)C(3)C(4)	101·1 (1)	101·2 (1)	C(9)C(10)C(11)	99·9 (2)	100·1 (2)
C(2)C(3)C(15)	114·2 (1)	112·0 (2)	C(7)C(11)C(10)	97·0 (2)	95·5 (1)
C(2)C(3)C(16)	111·9 (1)	112·8 (1)	C(1)C(12)C(4)	93·9 (1)	93·9 (1)
C(4)C(3)C(15)	111·9 (2)	111·0 (1)	C(2)C(13)N(13)	178·8 (5)	177·4 (3)
C(4)C(3)C(16)	108·8 (1)	111·8 (1)	C(2)C(14)N(14)	177·3 (3)	176·8 (4)
C(15)C(3)C(16)	108·7 (2)	108·0 (2)	C(3)C(15)N(15)	176·8 (2)	179·0 (7)
C(3)C(4)C(5)	108·2 (1)	108·4 (1)	C(3)C(16)N(16)	176·8 (3)	178·1 (3)
C(3)C(4)C(12)	100·3 (1)	100·2 (1)			
Interplanar angle	(1)*	(2)*	Interplanar angle	(1)*	(2)*
A–B	110·5	115·5	*D–F*	129·3	129·0
A–C	126·0	121·4	*E–F*	117·7	117·7
A–D	12·8	17·8	*G–E*	94·0	93·9
B–C	123·6	123·1	*H–E*	90·6	90·1
D–E	113·0	113·3	*G–H*	95·7	100·7

A = C(7)C(6)C(1)C(10), *B* = C(7)C(8)C(9)C(10), *C* = C(7)C(11)C(10),
D = C(1)C(4)C(5)C(6), *E* = C(1)C(2)C(3)C(4), *F* = C(1)C(12)C(4),
G = N(13)C(13)C(2)C(14)N(14), *H* = N(15)C(15)C(3)C(16)N(16)

* No deviation from least-squares plane greater than 0·02 Å. E.s.d.'s 0·6–0·8°.

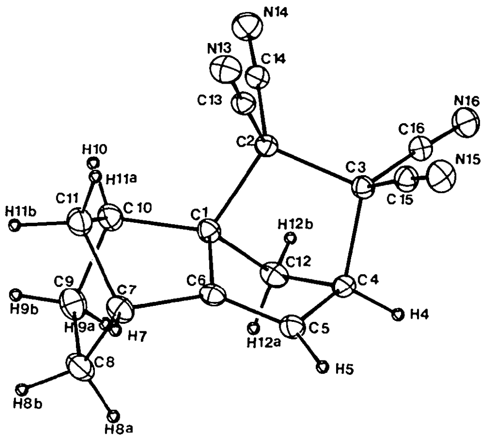

Fig. 1. *ORTEP* drawing of compound (1). Thermal ellipsoids are drawn at the 35% probability level.

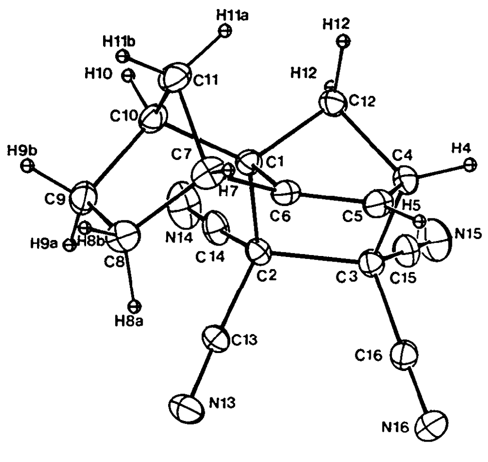

Fig. 2. *ORTEP* drawing of compound (2). Thermal ellipsoids are drawn at the 35% probability level.

N—C—C—C—N planes in each molecule form interplanar angles of 95·7 (5) and 100·7 (5)°. The average values for $C(sp^3)$—$C(sp)$ and C≡N of 1·475 (5) and 1·136 (4) Å in (1) and 1·473 (6) and 1·139 (3) Å in (2) are consistent with values from similar systems (Watson, Kashyap, Bartlett & Wu, 1984; Kashyap, Watson, Wu & Bartlett, 1984; Wang & Stucky, 1973; Karle, Flippen, Huisgen & Schug, 1975). The C(1)—C(2) bond lengths of 1·606 (3) and 1·601 (3) Å, the C(2)—C(3) lengths of 1·612 (2) and 1·620 (2) Å, and the C(3)—C(4) lengths of 1·577 (3) and 1·578 (3) Å in (1) and (2) are consistent with the lengthened bonds observed in the above references. The C(1)—C(2) and C(3)—C(4) lengths are not identical due to differences in interactions of the cyano groups.

The molecules can be considered to be composed of fused five-membered rings in envelope conformations or fused six-membered rings held in boat conformations by methylene bridges. The sixteen valence angles of less than 105° imply considerable ring strain within the molecules. There are no intermolecular contacts in compound (2) less than 2·60 Å but there are three in (1). The shortest contact of 2·37 Å is between H(4) of one molecule and H(8*a*) of another. Contacts between H(7′)···H(8*b*) and H(4′)···H(11*c*) are about 2·50 Å.

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Structure of 1,2-Dipiperidinoethane Mono-*N*-oxide Monoperchlorate Monohydrate,* $(C_{12}H_{25}N_2O)^+.ClO_4^-.H_2O$

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Abstract. $M_r = 330\cdot8$, monoclinic, $P2_1/n$, $a = 11\cdot366\ (2)$, $b = 6\cdot540\ (1)$, $c = 22\cdot082\ (3)$ Å, $\beta = 95\cdot52\ (1)$°, $V = 1633\cdot8\ (5)$ Å^3, $Z = 4$, $D_x = 1\cdot34$ Mg m^{-3}, Cu $K\alpha$, $\lambda = 1\cdot54178$ Å, $\mu = 2\cdot34$ mm^{-1}, $F(000) = 712$, room temperature, $R = 0\cdot062$ for 1892 observed reflexions. The organic cation is *cisoidal* with a very short intramolecular O···H···N hydrogen bond [O···N 2·551 (4) Å]. The H atom in this heteroatomic bridge appears to be more or less central. Water molecules and the cations are H bonded to form infinite chains in which the H_2O molecules are double donors and the N—O groups double acceptors.

Introduction. Our earlier investigations of the 1,1′-ethylenebis(piperidine 1-oxide) $[PEtP(NO)_2]$ system revealed that it prefers the *transoidal* conformation (Jaskólski, Kosturkiewicz, Mickiewicz-Wichłacz & Wiewiórowski, 1979; Jaskólski, 1982) unless it is monoprotonated in which case the *cisoidal* form is adopted with the two N—O functions linked by a very short O···H···O hydrogen bridge (Jaskólski, Gdaniec

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* *N*-(2-Piperidinoethyl)piperidinium *N*′-oxide perchlorate monohydrate.

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