Similar staggered synperiplanar conformations were observed in, for example, solid 4-*tert*-butyl-3,5-dinitroanisole (Van Havere, Lenstra & Geise, 1982), solid 5-*endo*-(bromomethyl)-1,2,4-trichloro-3,7,7-trimethoxynorborn-2-ene (Van Hemelrijk, Lenstra & Geise, 1982) and gaseous methyl vinyl ether (Durig & Compton, 1978; Pyckhout, Van Nuffel, Van Alsenoy, Van den Enden & Geise, 1983).

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References

CHATTERJEE, J. N., MUKHERJEE, J. & SENGUPTA, S. C. (1975). *Indian J. Chem.* **13**, 859–860.

CREMER, D. & POPLE, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.

DURIG, J. R. & COMPTON, D. A. (1978). *J. Chem. Phys.* **69**(5), 2028–2035.

FRENZ, B. A. (1978). *The Enraf–Nonius CAD-4 SDP.* In *Computing in Crystallography*, edited by H. SCHENK, R. OLTHOF-HAZEKAMP, H. VAN KONINGSVELD & G. C. BASSI, pp. 64–71. Delft Univ. Press.

GERMAIN, G., MAIN, P. & WOOLFSON, M. M. (1971). *Acta Cryst.* **A27**, 368–376.

GUPTA, M. P. & RAM, P. (1979). *Indian J. Phys.* **53A**, 474–476.

HAISGEN, R., SEIDL, G. & WIMMER, I. (1964). *Justus Liebigs Ann. Chem.* **677**, 21.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press.

LIPSON, H. & COCHRAN, W. (1966). *The Determination of Crystal Structures*, pp. 300 *ff.* London: Bell.

NORRESTAM, P. (1981). *Acta Cryst.* **A37**, 764–765.

PYCKHOUT, W., VAN NUFFEL, P., VAN ALSENOY, K., VAN DEN ENDEN, L. & GEISE, H. J. (1983). *J. Mol. Struct.* **102**, 333–345.

SPARKS, R. A. (1974). *Least-Squares Tutorial.* Proc. Am. Crystallogr. Assoc. Meet., Berkeley, California, pp. 99 *ff.*

VAN HAVERE, W., LENSTRA, A. T. H. & GEISE, H. J. (1982). *Acta Cryst.* **B38**, 3119–3120.

VAN HEMELRIJK, D., LENSTRA, A. T. H. & GEISE, H. J. (1982). *Acta Cryst.* **B38**, 2760–2763.

Structure of 4-Amino-*N*-2-pyridylbenzenesulphonamide (Sulphapyridine), C₁₁H₁₁N₃O₂S

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Abstract. $M_r = 249 \cdot 29$, monoclinic, $C2/c$, $a = 12 \cdot 807$ (3), $b = 11 \cdot 711$ (3), $c = 15 \cdot 379$ (2) Å, $\beta = 94 \cdot 07$ (2)°, $V = 2300 \cdot 8$ (9) Å³, $Z = 8$, $D_m = 1 \cdot 441$, $D_x = 1 \cdot 439$ Mg m⁻³, $F(000) = 1040$, Mo $K\alpha$, $\lambda = 0 \cdot 7107$ Å, $\mu = 0 \cdot 273$ mm⁻¹, $T = 298$ K, final $R = 0 \cdot 041$ for 2160 observed reflections. The molecule is found to exist as the imido tautomer. Its structural parameters are compared with those of other related molecules. In packing, centrosymmetrically related molecules dimerize through N–H⋯O hydrogen bonds; additional intra- and intermolecular N–H⋯O and N–H⋯N hydrogen bonds stabilize the structure. The pyridine and the phenyl rings stack independently.

Introduction. Sulphapyridine is an N^1-heteroaromatic sulphonamide used as an antibacterial drug in the treatment of pneumonia (Nitya Anand, 1979). The X-ray structural study of the compound has been carried out as part of our studies of N^1-substituted sulphonamides which we have undertaken with the view of correlating the structural features with the antibacterial activities (Basak, Mazumdar & Chaudhuri, 1982, 1983, 1984). Our study has shown that in the crystalline state the molecule exists as the imido tautomer $H_2N–C_6H_4SO_2N=C_5H_5N$. In addition, the molecular geometry and the conformation are compared with that of a structurally similar compound, ethyl 3-[4,5-dimethoxy-2-(4-methyl-2-pyridyl-sulphamoyl)phenyl]propionate (Eliopoulos, Sheldrick & Homodrakas, 1983).

Experimental. Crystals obtained from hot methanol and from acetone; crystals from acetone unstable. Density by flotation (KI solution). Space group Cc or $C2/c$ (hkl: $h+k =$ odd absent, $h0l$: l odd absent); ambiguity resolved by $N(z)$ test, E statistics and finally by successful refinement. Crystal $0 \cdot 30 \times 0 \cdot 30 \times 0 \cdot 35$ mm. Enraf–Nonius CAD-4 diffractometer, graphite-monochromatized Mo $K\alpha$. Lattice parameters from 25 reflections ($16° \leq \theta \leq 20°$). 2503 unique reflections ($2° \leq \theta \leq 27°$, $-16 \leq h \leq 16$, $0 \leq k \leq 14$, $0 \leq l \leq 19$), 2160 observed with $I \geq 3\sigma(I)$. Centring monitored after every 50 reflections (590, 0,2,14 and 6,2,12), intensity monitored after every hour of exposure (3,5,11, 596 and 2,4,13); data corrected for Lp and variation in intensity (<2%), absorption ignored. Direct methods

(*MULTAN*78; Main, Hull, Lessinger, Germain, De-clercq & Woolfson, 1978; 160 *E* values ≥ 1·6). Anisotropic full-matrix refinement based on *F* (*ORFLS*; Busing, Martin & Levy, 1962). H (from ΔF synthesis) isotropic. $R = 0·041$, $R_w = 0·041$, $S = 1·621$, $w = 1/\sigma^2(|F_o|)$. Max. $\Delta/\sigma < 0·01$. Peak heights in final ΔF map from $-0·17$ to $+0·21$ e Å^{-3}. Scattering factors for non-H atoms from Cromer & Waber (1965) and for H atoms from Stewart, Davidson & Simpson (1965). Anomalous-dispersion corrections for all non-H atoms from *International Tables for X-ray Crystallography* (1974).
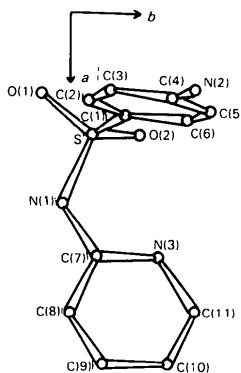

Fig. 1. View of the molecule down the *c* axis.

Table 1. *Fractional atomic coordinates and thermal parameters with e.s.d.'s in parentheses [equivalent isotropic temperature factors B_{eq}(Å^2) (Hamilton, 1959) for non-hydrogen atoms and isotropic temperature factors B(Å^2) for H atoms]*

	x	*y*	*z*	B_{eq}/B
S	0·20357 (5)	0·04272 (5)	0·56200 (4)	2·34
O(1)	0·1352 (2)	−0·0543 (1)	0·5429 (1)	3·21
O(2)	0·2027 (1)	0·1332 (1)	0·4968 (1)	2·81
N(1)	0·3186 (2)	−0·0101 (2)	0·5811 (1)	2·67
N(2)	0·1265 (2)	0·2350 (2)	0·9058 (2)	3·87
N(3)	0·4070 (2)	0·1703 (2)	0·5767 (2)	2·65
C(1)	0·1702 (2)	0·1030 (2)	0·6603 (1)	2·20
C(2)	0·1452 (2)	0·0313 (2)	0·7275 (2)	2·68
C(3)	0·1294 (2)	0·0745 (2)	0·8086 (2)	2·76
C(4)	0·1388 (2)	0·1924 (2)	0·8249 (2)	2·56
C(5)	0·1601 (2)	0·2641 (2)	0·7556 (2)	2·87
C(6)	0·1767 (2)	0·2206 (2)	0·6746 (2)	2·65
C(7)	0·4036 (2)	0·0558 (2)	0·5925 (2)	2·61
C(8)	0·5005 (2)	−0·0058 (3)	0·6232 (2)	3·81
C(9)	0·5873 (2)	0·0716 (3)	0·6371 (2)	4·93
C(10)	0·5848 (2)	0·1888 (3)	0·6211 (2)	4·57
C(11)	0·4937 (2)	0·2359 (3)	0·5905 (2)	3·55
H(2)	0·140 (2)	−0·053 (2)	0·715 (1)	2·8 (5)
H(3)	0·111 (2)	0·028 (2)	0·851 (1)	2·2 (5)
H(5)	0·161 (2)	0·343 (2)	0·766 (2)	3·9 (6)
H(6)	0·194 (2)	0·267 (2)	0·630 (1)	2·0 (5)
H(21)	0·126 (2)	0·188 (2)	0·950 (2)	4·4 (7)
H(22)	0·142 (2)	0·309 (3)	0·915 (2)	5·4 (9)
H(8)	0·500 (2)	−0·074 (2)	0·640 (2)	5·1 (7)
H(9)	0·486 (2)	0·317 (2)	0·577 (2)	4·3 (7)
H(10)	0·643 (2)	0·237 (2)	0·632 (2)	5·0 (8)
H(11)	0·650 (2)	0·038 (2)	0·655 (2)	5·2 (7)
H(30)	0·347 (2)	0·195 (3)	0·555 (2)	5·2 (1·1)

Table 2. *Bond distances (Å), bond angles (°), selected torsion angles (°) and hydrogen-bonding dimensions*

S—O(1)	1·443 (1)	S—O(2)	1·458 (1)
S—N(1)	1·605 (3)	S—C(1)	1·749 (2)
C(1)—C(2)	1·387 (3)	C(2)—C(3)	1·374 (4)
C(3)—C(4)	1·407 (3)	C(4)—C(5)	1·399 (4)
C(5)—C(6)	1·376 (4)	C(6)—C(1)	1·396 (3)
N(1)—C(7)	1·336 (3)	C(7)—C(8)	1·422 (4)
C(8)—C(9)	1·357 (4)	C(9)—C(10)	1·394 (5)
C(10)—C(11)	1·345 (4)	C(11)—N(3)	1·354 (4)
N(3)—C(7)	1·364 (3)	N(2)—C(4)	1·360 (5)
C(1)—C(2)—C(3)	120·7 (2)	C(2)—C(3)—C(4)	120·4 (2)
C(3)—C(4)—C(5)	118·2 (2)	C(4)—C(5)—C(6)	121·2 (2)
C(5)—C(6)—C(1)	119·8 (2)	C(6)—C(1)—C(2)	119·6 (2)
N(2)—C(4)—C(3)	120·6 (2)	N(2)—C(4)—C(5)	121·2 (2)
C(1)—S—O(1)	108·0 (1)	C(1)—S—O(2)	108·1 (1)
C(1)—S—N(1)	105·9 (1)	S—N(1)—C(7)	122·0 (2)
N(1)—S—O(1)	105·8 (1)	N(1)—S—O(2)	111·6 (1)
N(1)—C(7)—N(3)	125·5 (2)	N(1)—C(7)—C(8)	119·3 (2)
C(7)—C(8)—C(9)	120·3 (3)	C(8)—C(9)—C(10)	121·5 (3)
C(9)—C(10)—C(11)	118·3 (3)	C(10)—C(11)—N(3)	120·2 (3)
C(11)—N(3)—C(7)	124·5 (3)	N(3)—C(7)—C(8)	115·2 (2)
S—C(1)—C(2)	118·9 (2)	S—C(1)—C(6)	121·3 (2)
O(1)—S—O(2)	116·9 (1)		
C(6)—C(1)—S—O(1)	−145·4 (2)	[136·1 (4)]	
C(6)—C(1)—S—O(2)	−18·1 (2)	[10·5 (4)]	
C(2)—C(1)—S—O(1)	39·9 (2)	[−44·4 (4)]	
C(2)—C(1)—S—O(2)	167·2 (2)	[−170·0 (4)]	
C(6)—C(1)—S—N(1)	101·6 (2)	[−111·1 (4)]	
C(2)—C(1)—S—N(1)	−73·1 (2)	[68·5 (4)]	
C(1)—S—N(1)—C(7)	−72·5 (2)	[68·9 (4)]	
O(1)—S—N(1)—C(7)	173·0 (2)	[−176·0 (4)]	
O(2)—S—N(1)—C(7)	44·9 (2)	[−48·8 (4)]	
S—N(1)—C(7)—C(8)	169·7 (2)	[176·1 (3)]	
S—N(1)—C(7)—N(3)	−10·6 (4)	[−4·4 (7)]	

Hydrogen bonding [symmetry code: (i) $\frac{1}{2}-x$, $\frac{1}{2}+y$, $\frac{3}{2}-z$; (ii) x, $-y$, $\frac{1}{2}+z$; (iii) $\frac{1}{2}-x$, $\frac{1}{2}-y$, $1-z$]

A—H⋯B	A—H (Å)	A—B (Å)	H⋯B (Å)	$\angle A$—H⋯B (°)
N(2)—H(22)⋯N(1^i)	0·90 (3)	3·070 (3)	2·18 (3)	171 (3)
N(2)—H(21)⋯O(1^{ii})	0·87 (3)	2·991 (3)	2·12 (3)	170 (2)
N(3)—H(30)⋯O(2^{iii})	0·86 (3)	2·885 (3)	2·24 (3)	131 (3)
N(3)—H(30)⋯O(2)	0·86 (3)	2·844 (3)	2·12 (3)	140 (3)

O(2)⋯H(3)⋯O(2^{iii})	86 (1)°

Discussion. Fig. 1 shows the labelling scheme. The final atomic coordinates and isotropic temperature factors are in Table 1.* Intramolecular bond distances, angles and some selected torsion angles are listed in Table 2. The torsion angles for ethyl 3-[4,5-dimethoxy-2-(4-methyl-2-pyridylsulphamoyl)phenyl]propionate, computed from the published coordinates (Eliopoulos *et al.*, 1983), are given in square brackets. Their atomic labelling scheme has been changed to conform to that of ours.

The structure analysis reveals that in the crystalline state sulphapyridine exists as the imido tautomer with the amido H having migrated to the pyridine N. This is
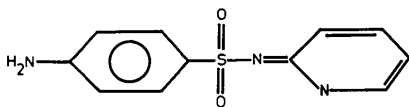
indicated by the actual location of the H atom in a difference Fourier synthesis, successful refinement of its parameters and the satisfactory geometry of the hydrogen bond involving it.

S has the usual distorted tetrahedral configuration (Alléaume, Gulko, Herbstein, Kapon & Marsh, 1976). The intramolecular contacts $O(1)\cdots O(2)$ [2·472 (2) Å], $O(1)\cdots N(1)$ [2·434 (3) Å] and $O(2)\cdots N(1)$ [2·535 (3) Å] observed in the present structure agree well with those found in dibenzenesulphonamide and its sodium salt (Cotton & Stokley, 1970), sulphacetamide {*N*-[(4-aminophenyl)sulphonyl]acetamide} (Basak *et al.*, 1982), sulphamethazine [4-amino-*N*-(4,6-dimethyl-2-pyrimidinyl)benzenesulphonamide] (Basak *et al.*, 1983) and sulphaproxyline (*p*-isopropoxy-*N*-sulphanilylbenzamide) (Basak *et al.*, 1984).

The observed shortening of the C(2)—C(3) and C(5)—C(6) bonds and narrowing of the C(3)—C(4)—C(5) angle in the phenyl ring from the expected values are due to substitution at the *para* position (Domenicano, Vaciago & Coulson, 1975) and has also been observed in other similar structures (Basak *et al.*, 1982, 1983, 1984; Kálmán, Czugler & Argay, 1981). The phenyl ring is not perfectly planar; deviations from planarity lie in the range +0·013 (3) Å to −0·018 (3) Å. The aryl amino nitrogen, N(2), and the S atom are, respectively, −0·060 (3) and −0·197 (1) Å away from the plane of the phenyl ring. The pyridine ring is almost planar; the deviations of the atoms from the least-squares plane lie in the range +0·006 (3) to −0·006 (3) Å. The dihedral angle between the least-squares planes of the two rings is 93·1 (1)°.

The short S—N(1) bond and the marked inequality in the two O—S—N angles indicate a two-coordinate N(1) atom consistent with the imido form of the compound (Kálmán, Czugler & Argay, 1981). The formal Lewis structure of the molecule can be written as follows:

The dihedral angle between the plane of the S,N(1) and C(7) atoms and the pyridine ring is 10·5°. The N(1)—C(7) bond distance is in agreement with N(sp^2)—C(sp^2) partial double-bond distances found in the sulphaguanidine molecule in its different crystalline forms (Alléaume *et al.*, 1976; Kálmán *et al.*, 1981). This, together with the lengthening of the C(7)—C(8) bond and narrowing of the endocyclic angle at C(7), indicates an extensive conjugation of the N(1)—C(7) bond with the pyridine ring.

The torsion angles about C(1)—S and S—N(1) bonds in the present structure as well as those in ethyl 3-[4,5-dimethoxy-2-(4-methyl-2-pyridylsulphamoyl)-phenyl]propionate are almost within the ranges for $|\varepsilon_1|$ and $|\varepsilon_2|$ quoted by Kálmán *et al.* (1981). It is observed that in spite of the marked differences in the substitution in the phenyl ring of the two molecules the conformations about the C(1)—S, S—N(1) and N(1)—C(7) bonds are similar, with maximum flexibility about the C(1)—S bond.

The crystal structure projected down the *b* axis is shown in Fig. 2. It is observed that the phenyl rings stack along the **a** direction while the pyridine rings stack along the **c** direction. This feature of stacking of like rings is somewhat similar to that observed in the crystal structure of sulphamethazine (Basak *et al.*, 1983).

The structure is stabilized by N—H⋯O and N—H⋯N hydrogen bonds. The aryl amino nitrogen, N(2), is the donor in an N—H⋯N(imido) bond to a screw-related molecule and an N—H⋯O(sulphonyl) bond to a glide-related molecule. The pyridine nitrogen, N(3), is the donor in a pair of bifurcated hydrogen bonds of the type N—H⋯O(sulphonyl), one intramolecular and the other intermolecular. The angle subtended at the hydrogen, H(30), by the two acceptors is 86 (1)° and is typical for such bifurcated hydrogen
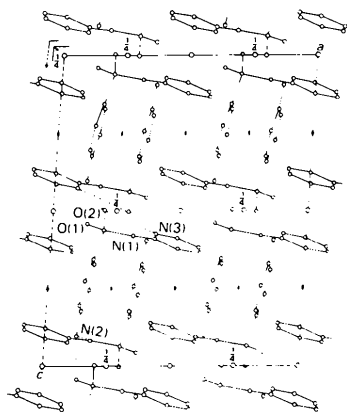

The C(7)—N(3)—C(11) bond angle is wider by about 5° than that reported (119·94°) for pyridine (Sørensen, Mahler & Rastrup-Anderson, 1974). Such widening of this endocyclic angle has been observed in a number of similar structures, where a hydrogen or a proton is attached to the pyridine N (Declercq, Schanck, Germain, Dereppe & Van Meerssche, 1977; Germain, Declercq, Schanck, Dereppe & Van Meerssche, 1977; Krajewski, Urbanczyk-Lipkowska & Gluzinski, 1977; Chandrasekhar, 1977; Bourne & Taylor, 1983). The C(7)—N(3) and N(3)—C(11) distances agree well with the values observed for other similar compounds (Eliopoulous *et al.*, 1983; Declercq *et al.*, 1977; Germain *et al.*, 1977; Krajewski *et al.*, 1977).

Fig. 2. Projection of the crystal structure of sulphapyridine down the *b* axis.

bonds (Jeffrey & Maluszynska, 1981). The intermolecular N—H···O hydrogen bonds link molecules related by centres of inversion, effectively resulting in a dimerization of the sulphapyridine molecules. One of the sulphonyl oxygens, O(2), is seen to accept two hydrogen bonds which, perhaps, explains the longer S—O bond length involving this O atom (Cotton & Stokley, 1970). The geometries of the hydrogen bonds are in Table 2.

References

ALLÉAUME, M., GULKO, A., HERBSTEIN, F. H., KAPON, M. & MARSH, R. E. (1976). Acta Cryst. B32, 669–682.

BASAK, A. K., MAZUMDAR, S. K. & CHAUDHURI, S. (1982). Cryst. Struct. Commun. 11, 1609–1616.

BASAK, A. K., MAZUMDAR, S. K. & CHAUDHURI, S. (1983). Acta Cryst. C39, 492–494.

BASAK, A. K., MAZUMDAR, S. K. & CHAUDHURI, S. (1984). Acta Cryst. C40, 419–422.

BOURNE, P. E. & TAYLOR, M. R. (1983). Acta Cryst. C39, 266–268.

BUSING, W. R., MARTIN, K. O. & LEVY, H. A. (1962). ORFLS. Report ORNL-TM-306. Oak Ridge National Laboratory, Tennessee.

CHANDRASEKHAR, K. (1977). Acta Cryst. B33, 143–145.

COTTON, F. A. & STOKLEY, P. F. (1970). J. Am. Chem. Soc. 92, 294–302.

CROMER, D. T. & WABER, J. T. (1965). Acta Cryst. 18, 104–109.

DECLERCQ, J.-P., SCHANCK, A., GERMAIN, G., DEREPPE, J. M. & VAN MEERSSCHE, M. (1977). Acta Cryst. B33, 3876–3877.

DOMENICANO, A., VACIAGO, A. & COULSON, C. A. (1975). Acta Cryst. B31, 221–234.

ELIOPOULOUS, E., SHELDRICK, B. & HOMODRAKAS, S. (1983). Acta Cryst. C39, 743–745.

GERMAIN, G., DECLERCQ, J.-P., SCHANCK, A., DEREPPE, J. M. & VAN MEERSSCHE, M. (1977). Acta Cryst. B33, 3878–3880.

HAMILTON, W. C. (1959). Acta Cryst. 12, 609–610.

International Tables for X-ray Crystallography (1974). Vol IV. Birmingham: Kynoch Press.

JEFFREY, G. A. & MALUSZYNSKA, H. (1981). Int. J. Quantum Chem. Quantum Biol. Symp. 8, 231–239.

KÁLMÁN, A., CZUGLER, M. & ARGAY, GY. (1981). Acta Cryst. B37, 868–877.

KRAJEWSKI, J., URBANCZYK-LIPKOWSKA, Z. & GLUZINSKI, P. (1977). Acta Cryst. B33, 2967–2969.

MAIN, P., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1978). MULTAN78. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data. Univs. of York, England, and Louvain, Belgium.

NITYA ANAND (1979). Burger's Medicinal Chemistry, Part II, edited by M. E. WOLFF, pp. i–40. New York: John Wiley.

SØRENSEN, G. O., MAHLER, L. & RASTRUP-ANDERSON, N. (1974). J. Mol. Struct. 20, 119–126.

STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). J. Chem. Phys. 42, 3175–3187.

rel-(5R,6R,9S,10S)-5,6,7,8,9,10-Hexahydro-2-phenyl-5,10:6,9-dimethano-1H-[1,2,4]triazolo[1,2-b]phthalazine-1,3(2H)-dione, C18H17N3O2

By RAM P. KASHYAP,* WILLIAM H. WATSON, CHENGJIU WU AND PAUL D. BARTLETT

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Abstract. $M_r = 307.33$, monoclinic, $P2_1/n$, $a = 9.439$ (2), $b = 19.454$ (8), $c = 8.382$ (3) Å, $\beta = 102.70$ (2)°, $V = 1501.4$ (9) Å^3, $Z = 4$, $D_x = 1.360$ g cm^{-3}, λ(Cu Kα) = 1.54178 Å, $\mu = 7.46$ cm^{-1}, $F(000) = 648$, room temperature, $R = 0.035$ for 1762 unique reflections with $I > 3\sigma(I)$. The central double bond in the anti-sesquinorbornene moiety is 1.327 (3) Å, and the C atoms are slightly pyramidalized. The pyramidalization leads to a 4.3 (4)° deviation from planarity. The phenyl group is planar, the five-membered triazolo ring has an envelope conformation.

Introduction. Although isodicyclopentadiene (1) prefers endo-face attack by many dienophiles to give Diels–Alder cycloadducts with the syn-sesquinorbornene

ring system (Sugimoto, Kobuke & Furukawa, 1976; Böhm, Carr, Gleiter & Paquette, 1980; Watson, Galloy, Bartlett & Roof, 1981), it is now found that the stereo course is reversed when more reactive dienophiles are used (Watson, Kashyap, Bartlett & Wu, 1984). To determine whether steric bulkiness or inherent reactivity governs the exo attack, the reaction of (1) with 4-phenyl-3H-triazole-3,5(4H)-dione (PTAD), (2), was studied. The reaction gave the single product (3) in good yield; however, the instability of (3) in solution prevented further chemical characterization. The present study demonstrates that the dienophile attacks from the exo face of the diene to form an anti-type cycloadduct. The structural data permit a comparison of contrasting theoretical approaches and yield parameters needed for the development of molecular mechanical computations on strained bicyclic systems.

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