valence angles and Fig. 1 is a drawing of the title compound.*

Related literature. The title compound was prepared from the reaction of diphenylfulvene and dichloroketene (Bartlett & Ando, 1970). The mechanism of hydrolysis of similar compounds to form tropolone derivatives has been reported (Asao, Machiguchi, Kitamura & Kitahara, 1970). Related crystal structures: Friedrichsen, Debaerdemaeker, Bottcher, Hahnemann & Schmidt (1983), Watson & Nagl (1987).

* Lists of H-atom coordinates, anisotropic thermal parameters and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44246 (20 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Acta Cryst. (1987). C43, 2465-2466

Structure of Bis(homoadamantane)

BY WILLIAM H. WATSON* AND ANTE NAGL[†]

Department of Chemistry, Texas Christian University, Fort Worth, Texas 76129, USA

(Received 24 June 1987; accepted 28 July 1987)

Abstract. 1,2,3,4,5,6,7,8,9,10,11,12,13,14-Tetradecahydro-1,5:3,7:8,12:10,14-tetramethanononalene

(eicosene) (1), $C_{20}H_{28}$, $M_r = 268.45$, monoclinic, $P2_1/n$, a = 6.593 (1), b = 12.114 (2), c = 9.628 (1) Å, $\beta =$ 92.19 (1)°, $V = 768.4 \text{ Å}^3$, Z = 2, $D_x = 1.16 \text{ g cm}^{-3}$, λ (Mo K α) = 0.71073 Å, μ = 0.60 cm⁻¹, F(000) = 296, T = 293 K, R = 0.054 for 968 unique reflections. The double bond is shielded on the ends by H...H separations of 2.05 (3) Å and on top and bottom by H····H separations ranging from 2.52 (3) to 3.14 (3) Å, which is consistent with the absence of normal olefinic reactivity in the molecule. Molecular-mechanics calculations predict $E_{\text{strain}} = 145.4 \text{ kJ}$ and $\Delta H_f =$ -77.6 kJ.



Experimental. Colorless crystal of (1); dimensions $0.45 \times 0.28 \times 0.30$ mm; Nicolet $R3m/\mu$ update of a P2, diffractometer; data collected in the Wyckoff mode $(3 \le 2\theta \le 50^\circ, \omega \text{ varied}, 2\theta \text{ fixed})$, variable scan speed (4 to 29.3° min⁻¹), monochromated Mo Ka radiation; lattice parameters from a least-squares refinement of 25

We thank the Welch Foundation (P-074), the National Science Foundation (CHE8514367) and the TCU Research Fund for financial support. We thank Professor Bartlett for the sample.

References

- Asao, T., Machiguchi, T., Kitamura, T. & Kitahara, Y. (1970). J. Chem. Soc. Chem. Commun. pp. 89-91.
- BARTLETT, P. D. & ANDO, T. (1970). J. Am. Chem. Soc. 92, 7518-7519.
- FRIEDRICHSEN, W., DEBAERDEMAEKER, T., BOTTCHER, A., HAHNEMANN, S. & SCHMIDT, R. (1983). Z. Naturforsch. Teil B, 38, 504-515.
- International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)
- Nicolet Instrument Corporation (1986). SHELXTL for Desktop 30 (Microeclipse), PN269-1040340, April.
- WATSON, W. H. & NAGL, A. (1987). Acta Cryst. Submitted.

Table 1. Atomic coordinates $(\times 10^4)$ and equivalent isotropic thermal parameters ($Å^2 \times 10^3$)

	x	у	Ζ	U_{eo}^*
C(1)	3 (3)	456 (2)	358 (2)	45 (1)
C(2)	-216(3)	475 (2)	1936 (2)	54 (1)
C(3)	-2267 (4)	36 (2)	2385 (2)	65 (1)
C(4)	-2407 (4)	-1205(2)	2408 (2)	64 (1)
C(5)	-714 (4)	-1663 (2)	3348 (2)	69 (1)
C(6)	1311 (4)	-1357 (2)	2754 (2)	71 (1)
C(7)	1515 (4)	-108(2)	2725 (2)	69 (1)
C(8)	-2293 (4)	-1732(2)	978 (2)	66 (1)
C(9)	1481 (4)	-1885 (2)	1340 (3)	71 (1)
C(10)	-249 (4)	-1587 (2)	315 (2)	56 (1)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ii} tensor.

reflections ($20.57 \le 2\theta \le 35.35^{\circ}$), angles measured by a centering routine associated with the diffractometer; systematic absences (h0l, h + l = 2n + 1; 0k0, k =2n + 1) consistent with space group $P2_1/n$, Laue symmetry 2/m; two monitored reflections (301 and $0\overline{13}$) showed no statistically significant changes in intensities; 1348 independent reflections measured $(0 \le h \le 7, 0 \le k \le 14, -11 \le l \le 11)$ with $968 \ge$ $3\sigma(I)$; Lorentz-polarization corrections applied, ψ -scan empirical absorption correction (transmission factors 0.903-0.977); direct methods and difference Fourier syntheses revealed the positions of all atoms; blockcascade least-squares refinement with a single thermal parameter for all H atoms; R = 0.0525, wR = 0.0500, 968 reflections and 134 parameters, R = 0.0771 for all

© 1987 International Union of Crystallography

^{*} Author to whom correspondence should be directed.

[†] On leave from Faculty of Technology, University of Zagreb, Zagreb, Yugoslavia.

Table 2. Bond	lengths	(A)) and va	lence	angle	2S (0)
---------------	---------	-----	----------	-------	-------	------	---	---

C(1)-C(2)	1.532 (3)	C(1)–C(1')	1.302 (4)
C(1)-C(10')	1.527 (3)	C(2) - C(3)	1.531 (3)
C(2) - C(7)	1.521 (3)	C(3) - C(4)	1.506 (3)
C(4) - C(5)	1.515 (3)	C(4)C(8)	1.521 (3)
C(5)-C(6)	1.518 (4)	C(6) - C(7)	1.519 (4)
C(6)-C(9)	1.512 (3)	C(8) - C(10)	1.524 (3)
C(9)-C(10)	1.523 (3)	C(10) - C(1')	1.527 (3)
C(2)-C(1)-C(1')	122.6 (2)	C(2)-C(1)-C(10')	115.0 (2
C(1') - C(1) - C(10')	122.4(2)	C(1) - C(2) - C(3)	113.1 (2
C(1) - C(2) - C(7)	113.1(2)	C(3) - C(2) - C(7)	110.6 (2)
C(2) - C(3) - C(4)	114.0(2)	C(3)-C(4)-C(5)	109.3 (2
C(3) - C(4) - C(8)	113.6 (2)	C(5)-C(4)-C(8)	109.0 (2
C(4) - C(5) - C(6)	108.9 (2)	C(5) - C(6) - C(7)	109.3 (2
C(5) - C(6) - C(9)	109.4 (2)	C(7)-C(6)-C(9)	113.3 (2
C(2)-C(7)-C(6)	114.0 (2)	C(4) - C(8) - C(10)	114.0 (2
C(6) - C(9) - C(10)	113.8 (2)	C(8)-C(10)-C(9)	110.7 (2)
C(8) - C(10) - C(1')	113.0 (2)	C(9) - C(10) - C(1')	113.5 (2)
	(-)		

1351 reflections, S = 1.622; $(\Delta/\sigma)_{max} = 0.010$, $(\Delta/\sigma)_{av} = 0.002$; largest peaks in the final difference map of +0.15 and -0.13 e Å⁻³; $\sum w(|F_o| - |F_c|)^2$ minimized with $w = [\sigma^2(F_o) + 0.000223F_o^2]^{-1}$; all computer programs supplied by Nicolet for Desktop 30 Micro-eclipse and Nova 4 configuration (Nicolet Instrument Corporation, 1986); atomic scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974). The X-ray parameters were used in a molecular-mechanics calculation (Allinger & Yuh, 1980). Table 1 lists atomic positional parameters and U_{eq} values while Table 2 lists interatomic distances and valence angles.* The structure and atomic numbering of (1) are shown in Fig. 1.

Related literature. The lack of chemical reactivity of bis(homoadamantane) with singlet oxygen and epoxidizing agents (Meijer & Wynberg, 1981) and with

* Lists of H-atom coordinates, anisotropic thermal parameters and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44287 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.



Fig. 1. Drawing of the title compound. Thermal ellipsoids are drawn at the 25% probability level. H atoms are represented by spheres of arbitrary size.

 Br_2-CCl_4 and other reagents (Gill & Hands, 1971) has been discussed. Gerson, Lopez, Akaba & Nelson (1981) investigated the ease of electron loss and the stability of the resulting cation.

We thank The Welch Foundation (P-074) and the TCU Research Fund for financial support. We thank Professor Paul Bartlett and Dr David Morton for the sample.

References

- ALLINGER, N. L. & YUH, Y. H. (1980). MM2 with MMPI subroutines for IBM PC. Updated by L. C. ROHREN (1984); adapted by J. J. GAJEWSKI & K. E. GILBERT from copy supplied by O. NELSON & C. SCOTT OWEN. Obtained from Serena Software, 489 Serena Lane, Bloomington, IN 47401, USA.
- GERSON, F., LOPEZ, J., AKABA, R. & NELSON, S. F. (1981). J. Am. Chem. Soc. 103, 6716-6722.
- GILL, G. B. & HANDS, D. (1971). Tetrahedron Lett. pp. 181-184.
- International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)
- MEIJER, E. W. & WYNBERG, H. (1981). Tetrahedron Lett. pp. 785-788.
- Nicolet Instrument Corporation (1986). *SHELXTL* for Desktop 30 (Microeclipse), PN269-1040340, April, 1986. Nicolet XRD Corporation, Cupertino, CA, USA.

Acta Cryst. (1987). C43, 2466-2468

N-(N'-Phenylsulfamoyl)oxazolidinone-2

Par Bernard Bonnaud, Robert Viani, Bernadette Agoh, Barbara Delaunay, Georges Dewinter et Jean-Louis Montero

Département de Physique, Université d'Abidjan, 04 BP 322, Abidjan 04, Côte d'Ivoire

ET JEAN-PIERRE AYCARD

Laboratoire de Chimie Organique Structurale, Université de Provence, 13397 Marseille CEDEX 13, France

(Reçu le 29 avril 1987, accepté le 29 juillet 1987)

Abstract. 2-Oxo-3-oxazolidinesulfonanilide, 96.59 (3)°, V = 1066 (4) Å³, Z = 4, $D_m = 1.50$ (2), $C_9H_{10}N_2O_4S$, $M_r = 242.29$, monoclinic, $P2_1/c$, $a = D_x = 1.510 \text{ Mgm}^{-3}$, $Mo K\bar{a}$ radiation, $\lambda = 0.7107$ Å, 11.217 (3), b = 7.653 (2), c = 12.503 (6) Å, $\beta = \mu = 2.53 \text{ mm}^{-1}$, F(000) = 504, T = 295 K, final R = 0.2123

0108-2701/87/122466-03\$01.50

© 1987 International Union of Crystallography