$S = 0.64$
2242 reflections
162 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F) + 0.0003F^2]$

Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å²)

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
N1	0.7732 (2)	0.5662 (1)	0.1626 (1)	0.045 (1)
C2	0.6869 (2)	0.6186 (2)	0.1002 (1)	0.047 (1)
C3	0.7931 (2)	0.5466 (2)	0.0444 (1)	0.052 (1)
C4	0.8657 (2)	0.4207 (2)	0.0770 (1)	0.053 (1)
C5	0.9303 (2)	0.4708 (2)	0.1441 (1)	0.049 (1)
C6	0.4591 (2)	0.5961 (2)	0.1014 (1)	0.053 (1)
O7	0.3676 (2)	0.6608 (1)	0.0468 (1)	0.060 (1)
O8	0.9675 (2)	0.6166 (1)	0.0212 (1)	0.062 (1)
C9	1.0233 (3)	0.3422 (2)	0.0396 (1)	0.070 (2)
C10	0.8455 (2)	0.6648 (2)	0.2098 (1)	0.049 (1)
C11	0.6774 (3)	0.7594 (2)	0.2301 (1)	0.072 (2)
C12	0.9293 (2)	0.5995 (1)	0.2711 (1)	0.050 (1)
C13	0.8126 (3)	0.5117 (2)	0.3070 (1)	0.068 (2)
C14	0.8872 (5)	0.4572 (2)	0.3648 (1)	0.089 (3)
C15	1.0751 (5)	0.4897 (2)	0.3873 (1)	0.094 (3)
C16	1.1954 (4)	0.5758 (3)	0.3519 (1)	0.084 (2)
C17	1.1210 (3)	0.6302 (2)	0.2936 (1)	0.061 (2)

Table 2. *Selected geometric parameters* (Å, °)

N1—C2	1.484 (2)	C3—O8	1.434 (2)
N1—C5	1.471 (2)	C4—C5	1.513 (2)
N1—C10	1.468 (2)	C4—C9	1.515 (3)
C2—C3	1.519 (2)	C6—O7	1.421 (2)
C2—C6	1.520 (2)	C10—C11	1.528 (3)
C3—C4	1.525 (2)	C10—C12	1.513 (2)
C2—N1—C5	107.1 (1)	C3—C4—C9	116.6 (1)
C2—N1—C10	115.3 (1)	C5—C4—C9	115.8 (1)
C5—N1—C10	113.1 (1)	N1—C5—C4	104.8 (1)
N1—C2—C3	106.2 (1)	C2—C6—O7	109.7 (1)
N1—C2—C6	108.1 (1)	N1—C10—C11	112.0 (1)
C3—C2—C6	113.1 (1)	N1—C10—C12	110.3 (1)
C2—C3—C4	103.5 (1)	C11—C10—C12	108.9 (1)
C2—C3—O8	111.7 (1)	C10—C12—C13	120.8 (1)
C4—C3—O8	108.2 (1)	C10—C12—C17	120.3 (1)
C3—C4—C5	100.9 (1)		
C5—N1—C2—C3	2.3 (1)	C4—C5—N1—C2	−27.1 (1)
N1—C2—C3—C4	23.1 (1)	C2—N1—C10—C12	179.9 (2)
C2—C3—C4—C5	−38.6 (1)	N1—C10—C12—C13	−54.9 (2)
C3—C4—C5—N1	40.7 (1)	N1—C2—C6—O7	172.0 (2)

The parameters for the H atoms bonded to the hydroxy groups O7 and O8 were refined. The isotropic displacement factors of H atoms bonded to C atoms were set equal to $1.1U_{\rm eq}$ of the bonded atom. Two reflections, 340 and 002, were omitted from the refinement.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1987). Data reduction: *NONIUS* (Riche, 1989). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELX*76 (Sheldrick, 1976). Molecular graphics: *R3M* (Riche, 1983) and *ORTEP* (Johnson, 1965). Software used to prepare material for publication: *ACTACIF* (Riche, 1992).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AB1230). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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9,9′-Thiobis(1,2,3,4,7,8-hexahydro-7-methyl-6*H*-pyrimido[1,6-*a*]pyrimidine-6,8-dione)

VIKTOR KETTMANN

Department of Analytical Chemistry, Faculty of Pharmacy, Comenius University, Odbojárov 10, 83232 Bratislava, Slovakia

ALENA BOZÓOVÁ AND ALFONZ RYBÁR

Institute of Chemistry, Centre for Chemical Research, Slovak Academy of Sciences, Dúbravská cesta, 84238 Bratislava, Slovakia

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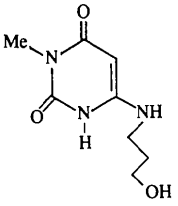
Abstract

The structure determination of $C_{16}H_{20}N_6O_4S$, has shown that the molecule consists of two fused-ring systems joined by an S atom. Each ring system is nearly planar except for one sp^3 C atom. The mean S—C distance [1.730 (3) Å] represents a bond order of 1.5. The bonding pattern of the pyrimidine-2,6-dione moiety is analysed in detail and compared with that of analogous compounds. The molecule is stabilized by two intramolecular hydrogen bonds, while the intermolecular packing is governed by van der Waals forces.

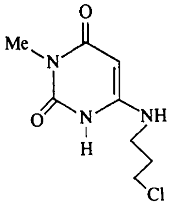
Comment

As a part of our studies on purine and pyrimidine derivatives, we attempted to convert, by treatment with thionylchloride, 6-(γ-hydroxypropylamino)-

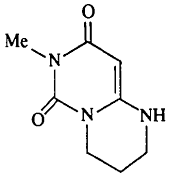
3-methyl-(1*H*,3*H*)-pyrimidine-2,6-dione, (1), to the corresponding 6-(γ-chloropropylamino) derivative (2), which, after cyclization, would give (3). However, spectroscopic and analytical data of the product were consistent with the structure (4), *i.e.* an additional reaction leading to the formation of the sulfide had occurred. To confirm this and, at the same time, to unravel the detailed stereochemistry of this compound, the crystal structure of (4) was determined by X-ray diffraction.



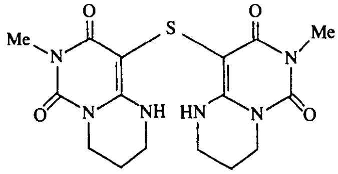
(1)



(2)



(3)



(4)

The ring system of the molecule comprises a methyl-substituted pyrimidine-2,6-dione moiety joined to a saturated hexahydropyrimidine ring; two such fused rings are linked by a sulfur bridge. One of the two independent ring systems (denoted *A* and *B*) exhibits positional disorder at atom C(5). While the two dioxo-methyl-substituted rings are nearly planar [the maximum out-of-plane deviations are 0.045 (3) and 0.054 (2) Å in the *A* and *B* ring systems, respectively], each saturated ring has an approximate sofa conformation with C(51)/C(52) (ring system *A*) and C(13) (ring system *B*) on the flap; deviations of the out-of-plane atom from the best plane of the remaining five atoms are 0.560 (7), 0.428 (7) and 0.631 (4) Å for C(51), C(52) and C(13), respectively. Obviously, the disorder of the C(5) atom results from inversion of the *A* ring. Analysing the conformations of the saturated rings in more detail (Cremer & Pople, 1975), the conformation of the ring in the *A* system can be described as intermediate between boat and twist-boat, whereas in *B* it is nearer a half chair. Apart from these ring puckers, both the *A* and *B* ring systems are almost planar.

Examination of compounds incorporating the pyrimidine-2,6-dione fragment has revealed that the bond lengths within this moiety assume different values in different derivatives, depending on the chemical environments resulting from the nature of the substituents (Everaert, Peeters, Blaton & De Ranter, 1990; McMullan & Craven, 1989; El Couhen, Courseille, Precigoux, Constant & Lhomme, 1983; Warin, Lobry, Baert, Bernier & Henichart, 1979; Stålhandske, Bruins Slot & Beurskens, 1985). In (4), the C(7)—N(3) bond is significantly shorter than the C(7)—N(2) bond (Table 2), which indicates extensive π delocalization along the chain N(3)—C(7)—C(1)—C(2)—O(1), where all the bonds have partial double-bond character. A similar bonding pattern is observed for the chemically equivalent portion of the *B* ring system and is also a characteristic of derivatives having a five- or six-membered heteroring joined to the pyrimidine-2,6-dione moiety at the double bond (Warin, Lobry, Baert, Bernier & Henichart, 1979; Stålhandske, Bruins Slot & Beurskens, 1985).

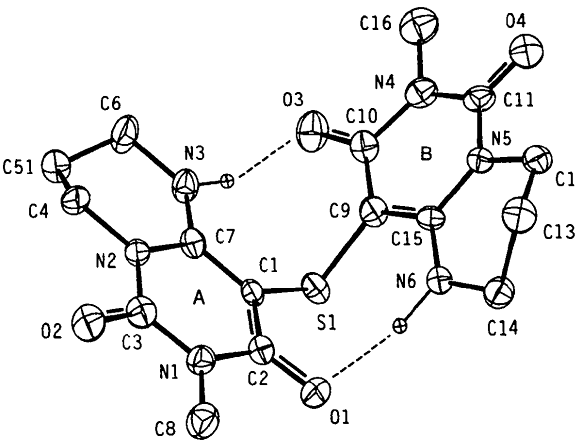


Fig. 1. A perspective view of the title molecule with atom numbering. Displacement ellipsoids are drawn at the 40% probability level. For clarity, only polar H atoms involved in intramolecular hydrogen bonds (dashed lines), are drawn. C(51) is one of the two disordered sites for atom C(5).

The torsion angles about the two S—C bonds of the sulfur bridge are 78.1 (3) and 79.0 (3)°. As a result, the dihedral angle between the mean planes of the unsaturated rings is 63.5 (2)°. The two S—C distances are 1.732 (3) and 1.729 (3) Å, which correspond to a bond order of 1.5 (Abrahams, 1956), assuming values of 1.82 and 1.61 Å for single S—C and double S=C bond lengths, respectively. This is in good agreement with the corresponding values found in a variety of 1-thiapyrane and thiophene derivatives (Banerjee, Brown & Jain, 1985; Kemmish & Hamor, 1988; Dillen, 1990). All these facts suggest that the lone electron pairs of the S atom could conjugate with the π system of the pyrimidine-2,6-dione moiety.

There are two intramolecular contacts shorter than the sum of the van der Waals radii: between the NH N atom and the carbonyl O atom (Table 2, Fig. 1). Although the N···O distances are somewhat larger than are usually found for hydrogen bonds, the H atoms lie approximately in the directions of the sp^2 lone pairs of the O atom so that these contacts may be regarded as intramolecular hydrogen bonds (Taylor, Kennard & Versichel, 1983). The packing of the molecules is governed by van der Waals forces.

Experimental

Crystals of the title compound were obtained by crystallization from ethanol/water. The crystal density D_m was measured by flotation in bromine/cyclohexane.

Crystal data

$C_{16}H_{20}N_6O_4S$
$M_r = 392.4$
Orthorhombic
*Fdd*2
$a = 23.875\ (11)$ Å
$b = 22.954\ (10)$ Å
$c = 11.877\ (5)$ Å
$V = 6509\ (3)$ Å^3
$Z = 16$
$D_x = 1.601$ Mg m^{-3}
$D_m = 1.60\ (1)$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 15 reflections
$\theta = 6$–$18°$
$\mu = 0.23$ mm^{-1}
$T = 293$ K
Prism
0.50 × 0.20 × 0.15 mm
Colourless

Data collection

Syntex $P2_1$ diffractometer
$\theta/2\theta$ scans
Absorption correction: none
3288 measured reflections
1515 independent reflections
1222 observed reflections [$I > 2\sigma(I)$]
$R_{\rm int} = 0.024$

$\theta_{\rm max} = 25°$
$h = 0 \rightarrow 28$
$k = 0 \rightarrow 27$
$l = 0 \rightarrow 14$
2 standard reflections monitored every 100 reflections frequency: 100 min intensity decay: 4%

Refinement

Refinement on F
$R = 0.052$
$wR = 0.055$
$S = 1.45$
1222 reflections
253 parameters
H-atom parameters not refined

$w = 1/[\sigma^2(F_o) + 0.0009|F_o|^2]$
$(\Delta/\sigma)_{\rm max} = 0.09$
$\Delta\rho_{\rm max} = 0.21$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.23$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$B_{\rm eq} = (4/3)\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	$B_{\rm eq}$
S(1)	−0.2395 (1)	0.4898 (1)	0.5855 (1)	3.85 (2)
O(1)	−0.3423 (1)	0.5620 (1)	0.6324 (2)	5.32 (7)
O(2)	−0.3878 (1)	0.4753 (1)	0.9586 (2)	4.68 (6)
N(1)	−0.3645 (1)	0.5196 (1)	0.7977 (2)	3.81 (7)
N(2)	−0.3210 (1)	0.4333 (1)	0.8548 (2)	3.14 (6)
N(3)	−0.2482 (1)	0.3934 (1)	0.7517 (2)	3.93 (7)
C(1)	−0.2896 (1)	0.4816 (1)	0.6897 (2)	2.94 (8)
C(2)	−0.3315 (1)	0.5225 (1)	0.6991 (3)	3.71 (9)
C(3)	−0.3595 (1)	0.4765 (1)	0.8723 (3)	3.59 (9)
C(4)	−0.3213 (1)	0.3847 (1)	0.9312 (3)	4.03 (10)
C(51)	−0.2665 (3)	0.3586 (3)	0.9405 (6)	3.86 (17)
C(52)	−0.2879 (3)	0.3340 (3)	0.8858 (6)	5.01 (23)
C(6)	−0.2406 (2)	0.3455 (2)	0.8252 (3)	5.58 (12)
C(7)	−0.2858 (1)	0.4361 (1)	0.7632 (3)	3.16 (8)
C(8)	−0.4055 (2)	0.5639 (1)	0.8198 (3)	5.26 (11)
O(3)	−0.1880 (1)	0.3735 (1)	0.5366 (2)	5.42 (8)
O(4)	−0.2779 (1)	0.3407 (1)	0.2124 (2)	4.86 (7)
N(4)	−0.2313 (1)	0.3584 (1)	0.3717 (3)	4.05 (8)
N(5)	−0.3074 (1)	0.4152 (1)	0.3168 (2)	3.09 (6)
N(6)	−0.3299 (1)	0.4986 (1)	0.4157 (2)	3.72 (7)
C(9)	−0.2556 (1)	0.4403 (1)	0.4807 (3)	3.69 (8)
C(10)	−0.2225 (1)	0.3910 (1)	0.4698 (3)	3.75 (9)
C(11)	−0.2720 (1)	0.3699 (1)	0.2946 (3)	3.69 (9)
C(12)	−0.3543 (1)	0.4210 (1)	0.2408 (3)	3.61 (9)
C(13)	−0.3980 (1)	0.4588 (2)	0.2911 (3)	4.91 (10)
C(14)	−0.3731 (1)	0.5145 (1)	0.3379 (3)	4.51 (10)
C(15)	−0.2973 (1)	0.4519 (1)	0.4048 (3)	3.08 (8)
C(16)	−0.1941 (1)	0.3091 (2)	0.3496 (4)	5.74 (12)

Table 2. *Selected geometric parameters* (Å, °)

S(1)—C(1)	1.732 (3)	S(1)—C(9)	1.729 (3)
C(1)—C(2)	1.376 (4)	C(9)—C(10)	1.385 (4)
C(2)—O(1)	1.233 (4)	C(10)—O(3)	1.212 (4)
C(2)—N(1)	1.413 (5)	C(10)—N(4)	1.402 (5)
N(1)—C(3)	1.332 (4)	N(4)—C(11)	1.360 (4)
C(3)—O(2)	1.227 (4)	C(11)—O(4)	1.192 (4)
C(3)—N(2)	1.368 (4)	C(11)—N(5)	1.366 (4)
N(2)—C(7)	1.376 (4)	N(5)—C(15)	1.365 (4)
C(7)—C(1)	1.363 (4)	C(15)—C(9)	1.370 (5)
N(2)—C(4)	1.438 (4)	N(5)—C(12)	1.445 (4)
N(3)—C(6)	1.415 (5)	N(6)—C(14)	1.433 (5)
N(3)—C(7)	1.337 (4)	N(6)—C(15)	1.329 (4)
C(1)—S(1)—C(9)	106.7 (2)	C(10)—N(4)—C(11)	124.2 (3)
C(2)—N(1)—C(3)	122.5 (3)	C(10)—N(4)—C(16)	118.1 (3)
C(2)—N(1)—C(8)	119.9 (3)	C(11)—N(4)—C(16)	117.6 (3)
C(3)—N(1)—C(8)	117.3 (3)	C(11)—N(5)—C(12)	115.5 (3)
C(3)—N(2)—C(4)	117.6 (3)	C(11)—N(5)—C(15)	120.6 (3)
C(3)—N(2)—C(7)	119.8 (3)	C(12)—N(5)—C(15)	123.9 (3)
C(4)—N(2)—C(7)	122.5 (3)	C(14)—N(6)—C(15)	124.3 (3)
C(6)—N(3)—C(7)	126.4 (3)		

D—H···A	D—H	H···A	D···A	D—H···A
N(6)—H···O(1)	1.05	1.96	2.972 (4)	161
N(3)—H···O(3)	0.86	2.15	2.967 (4)	160

The H atoms of the disordered saturated rings were not located.

Data collection: Syntex $P2_1$ diffractometer software. Cell refinement: Syntex $P2_1$ diffractometer software. Data reduction: *XP*21 (Pavelčík, 1987). Program(s) used to solve structure: *NRC* (Ahmed & Singh, 1973). Program(s) used to refine structure: *NRC*.

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: KA1042). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1995). C**51**, 1864–1868

1-Diisopropylphosphino-2-methyl-1,2-dicarba-*closo*-dodecaborane(12), (1), and 1,2-Bis(diisopropylphosphino)-1,2-dicarba-*closo*-dodecaborane(12), (2), at 193 K

RAIKKO KIVEKÄS

Inorganic Chemistry Laboratory, PO Box 6, FIN-00014 University of Helsinki, Finland

REIJO SILLANPÄÄ

Department of Chemistry, University of Turku, FIN-02500 Turku, Finland

FRANCESC TEIXIDOR, CLARA VIÑAS, ROSARIO NUÑEZ AND MAR ABAD

Departament de Quìmica, Universitat Autónoma de Barcelona and Institut de Ciència dels Materials, (CSIC), Campus de Bellaterra, 08193 Bellaterra, Barcelona, Spain

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Abstract

In the title compound (1), $C_9H_{27}B_{10}P$, the methyl and diisopropylphosphine groups are bonded to the C atoms of the 1,2-dicarbaborane cage. Bond lengths in (1) are P—C(cage) 1.876 (6) Å and C(cage)—C(cage) 1.731 (9) Å. In the 1,2-bis(diisopropylphosphine)-substituted carborane (2), $C_{14}H_{38}B_{10}P_2$, the P—C(cage) distances are 1.894 (3) and 1.891 (3) Å, and the C(cage)—C(cage) distance is 1.719 (3) Å. In both compounds, the P atoms are shifted from their expected positions towards the other cluster C atom resulting in low values of the P—C(cage)—C(cage) angles.

Comment

Computational studies on 1,2-dithioether-substituted 1,2-dicarba-*closo*-dodecaboranes, or *o*-carboranes, using semi-empirical quantum-mechanical calculations (CNDO, MNDO) suggest extremely long C—C distances. This implies that, to quantify HOMO–LUMO caps or other electronic properties, these otherwise useful calculations are not feasible unless the molecular parameters (distances and angles) are precisely known. To overcome this difficulty we propose that the C—C distances in *o*-carborane derivatives can be empirically derived from:

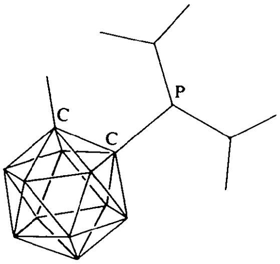
$$d = d_o + \Sigma a_i + \Sigma S_i$$

where d is the C—C distance in the carborane derivative, d_o the C—C distance [1.634 (3) Å] in C-non-substituted *o*-carborane (Šubrtová, Línek & Hasek, 1980), a_i is the additive electronic contributions and S_i the additive steric contributions.

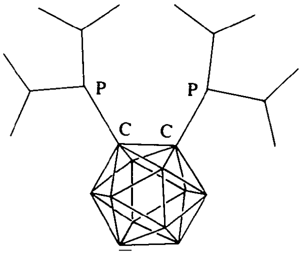
In order to ascertain the a_i and S_i values it is necessary to synthesize many carborane derivatives, incorporating various types of C substituents, and solve their crystal structures. For this purpose, we synthesized the title compounds (1) and (2). Unfortunately, we have not been able to obtain good crystals of (1) despite many attempts. Though the data quality of (1) is modest and the obtained bond parameters not as accurate as those of (2), the data it produces are significant both from a qualitative viewpoint and for use in semi-empirical methods. If the above equation is rewritten as

$$d = d_o + \Sigma(a_i + S_i)$$

the total contribution to the C—C bond distance of every radical can be estimated. Although the C—C distances in (1) and (2) are used with care, it appears that the —CH_3 contribution to the C—C distance is comparable to that of the $P[CH(CH_3)_2]_2$ group. This may suggest similar orbital contributions of both fragments to the cluster's cohesion, which could imply a simple σ-bond interaction. The reasonably good agreement between experimental and semi-empirically calculated results for phosphine-substituted *o*-carborane derivatives supports this hypothesis. To the contrary, large discrepancies have been found when S-substituted fragments are bonded to *o*-carborane. In that case other interactions besides the σ bonding may take place.



(1)



(2)

In (1) the P atom is bonded in a pyramidal arrangement to two C atoms of two isopropyl groups and to the C(1) atom of the carborane moiety. The P—C bond lengths are equal within experimental error. In 1-diphenylphosphino-2-methyl-1,2-dicarba-*closo*-dodecaborane, (3) (Kivekäs, Sillanpää, Teixidor, Viñas & Nuñez, 1994), and 1-diphenylphosphino-1,2-dicarba-*closo*-dodecaborane, (4) (Kivekäs, Teixidor, Viñas & Nuñez, 1995), the P—C(cage) distances agree with that