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2,2', 4,4', 6,6' - HEXAMETHYL - BIS - 4,4' - (4H) - PYRANE, C<sub>16</sub>H<sub>22</sub>O<sub>2</sub>

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#### PRELIMINARY INFORMATION

The title compound results from the action of strong organic reducing agents on the 2,4,6-trimethyl pyrylium cation (Conrow and Radlick, 1961). The substance is very non-polar and the two bipyran rings are linked by a single bond. NMR and spectroscopic measurements failed to prove unambiguously the exact nature of the molecule.

#### CRYSTAL DATA

(From Weissenberg photographs and single crystal diffractometry, CuK $\alpha$  = 1.5418 Å) Monoclinic, a = 7.838(4), b = 11.531(5), c = 8.846(4) Å,  $\beta$  = 113.56(2)<sup>o</sup>, Dx = 1.12 g cm<sup>-3</sup> for Z = 2; systematic absences for 0k0 reflexions with k = 2n+1 and for h0l reflexions with l = 2n+1, space group P2<sub>1</sub>/C.

#### INTENSITY DATA, STRUCTURE DETERMINATION AND REFINEMENT

The integrated intensities of 655 unique reflections were measured on an automatic four-circle Hilger and Watts diffractometer controlled by a PDP8 computer. The structure was solved with MULTAN (Main, 1980).

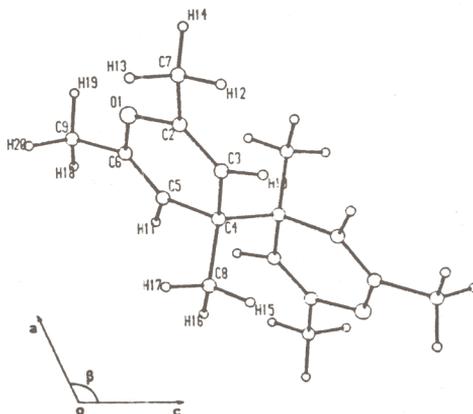
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The E-map calculated from the set of phases with the highest combined figure of merit (3.0) showed all the 9 non-hydrogen atoms. The refinement was by full-matrix least squares, using anisotropic temperature factors for all the individual atoms. Hydrogen atoms were assigned isotropic factors and the methyl groups were refined as rigid groups. The final R-factor was 11%.

ATOMIC CO-ORDINATES AND STANDARD DEVIATIONS ( $\times 10^4$ )

	X/A	Y/B	Z/C
O1	8046(5)	5908(3)	3278(4)
C2	7689(7)	6599(4)	4392(6)
C3	6343(8)	6389(5)	4858(7)
C4	4940(7)	5383(5)	4253(6)
C5	5605(9)	4669(5)	3100(7)
C6	6984(7)	4931(4)	2703(6)
C7	8970(8)	7595(5)	4879(7)
C8	2938(6)	5827(5)	3305(6)
C9	7493(8)	4312(5)	1482(6)



The molecule viewed along the  $[010]$  direction and numbering scheme of atoms

INTERATOMIC DISTANCES AND STANDARD DEVIATION (Å)

O1 - C2	1.380(6)	C4 - C5	1.554(7)
O1 - C6	1.372(6)	C4 - C8	1.542(7)
C2 - C3	1.300(7)	C4 - C4'	1.560(9)
C2 - C7	1.472(7)	C5 - C6	1.299(7)
C3 - C4	1.540(8)	C6 - C9	1.476(7)

INTERATOMIC ANGLES AND STANDARD DEVIATION (°)

C2 - O1 - C6	118.2(4)	C5 - C4 - C8	110.7(5)
O1 - C2 - C3	122.7(5)	C5 - C4 - C4'	109.3(5)
O1 - C2 - C7	110.5(4)	C8 - C4 - C4'	110.8(6)
C3 - C2 - C7	126.7(5)	C4 - C5 - C6	126.0(5)
C2 - C3 - C4	126.0(5)	O1 - C6 - C5	122.5(5)
C3 - C4 - C5	104.3(4)	O1 - C6 - C9	111.5(4)
C3 - C4 - C8	111.7(5)	C5 - C6 - C9	125.7(5)
C3 - C4 - C4'	109.6(6)		

COMMENTS

The molecule lies on the centre of symmetry. Moreover, the molecule has its own symmetry,  $2/m$  with two fold axis nearly parallel to  $[122]$  direction. R.M.S. deviation of atomic positions from the  $2/m$  symmetry is about  $0.01 \text{ \AA}$ . The pyrane ring is planar, the maximum displacement being about  $0.04 \text{ \AA}$  for O atom from the best plane passing through all the other atoms of the ring.

ACKNOWLEDGEMENT

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