Fig. 2. Packing of molecules projected on (001). (Distances in Å.)

Previous studies on the conformational properties of selective α_1- and α_2-antagonists have shown that there are at least two sites involved in the binding of these drugs to their adrenoceptors: a protonated nitrogen (at physiological pH) and an area rich in electrons (which is in most cases an aromatic system). See, for instance, the structure of WB-4101 {N-[2-(2,6-dimethoxy-phenoxy)ethyl]-1,4-benzodioxane-2-methylamine} (Carpy, Colleter & Léger, 1981), which is a selective α_1-antagonist, and the structure of BE-2254 {3,4-dihydro-2-[(p-hydroxyphenethyl)aminomethyl]-1(2H)-naphthalenone} (Carpy, Léger & Colleter, 1984), which is a selective α_2-antagonist. In all cases, the distance between these two sites is close to 5·5 Å. In the present compound, the protonated nitrogen is N(9) and the area rich in electrons is represented by the sulphon-

amide group. The calculated distance between N(9) and S(16) is 5·57 (1) Å.

The crystalline cohesion is ensured by a hydrogen bond involving N(9)+ and Cl(23)− ions: N(9)···Cl(23) $(-1 + x,\ y,\ 1 + z) = 3\cdot037$ (3) Å, H(109)···Cl(23) $= 2\cdot04$ (4) Å, N(9)—H(109)···Cl(23) $= 177$ (3)°, and by van der Waals contacts (Fig. 2).

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(2,5-Dimethoxy-3-cyclopenten-1-yl)dimethyl(2-propenyl)ammonium Iodide, $C_{12}H_{22}NO_2^+.I^-$

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Abstract. $M_r = 339\cdot2$, monoclinic, $P2_1/c$, $a = 10\cdot233$ (4), $b = 14\cdot005$ (8), $c = 11\cdot013$ (6) Å, $\beta = 99\cdot12$ (4)°, $V = 1558$ (2) Å^3, $Z = 4$, $D_x = 1\cdot446$ Mg m^{-3}, Mo $K\alpha$, $\lambda = 0\cdot71069$ Å, $\mu = 20\cdot72$ cm^{-1}, $F(000) = 688$, $T = 297$ K, m.p. = 435–436 K, $R = 0\cdot031$, $R_w = 0\cdot036$ for 1462 reflections.

The molecule, an N-allyl-N-cyclopentenyldimethyl-ammonium iodide, has two chiral centers in the cyclopentene ring. It is achiral, however, because of an internal plane of symmetry that bisects the cyclopentene π bond. The iodide ion, which lies almost on an extension of the cyclopentene-to-nitrogen bond, has

three hydrogen atoms closer than 3·2 Å. The nitrogen is *trans* to the two symmetrically placed oxygens of the methoxy ring substituents.

Introduction. Photochemical transformation of organic molecules often leads to interesting products *via* predictable pathways. In some cases, however, unusual processes occur for systems with unusual chromophores. An example of this is found in the photochemistry of the *N*-prenyl- and *N*-allylpyridinium perchlorates (I) and (III). The *N*-prenyl efficiently photoconverts to the hexahydroindolizine (II) by electron transfer, but the slightly smaller *N*-allyl salt (with hydrogens replacing two methyls) yields the much different cyclopentenylamine (IV). The unusual structure of photoproduct (IV) was elucidated by X-ray crystallography on its dimethylammonium salt derivative, (V). Details of the preparation of (V) and a general discussion of the photochemistry of these and related systems are given by Yoon, Quillen, Mariano, Swanson, Stavinoha & Bay (1983).

(I)   (II)

(III)   (IV)

(V)
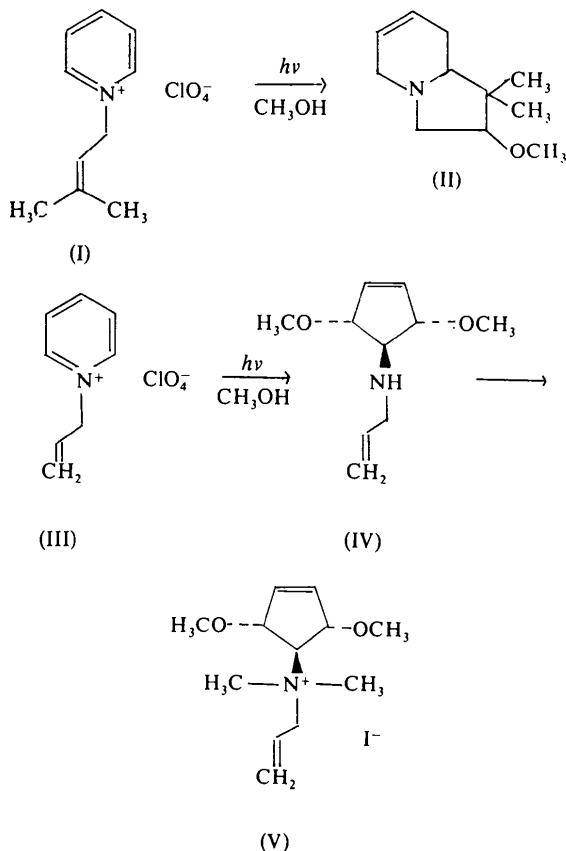
Experimental. Plate-shaped crystal, 0·3 × 0·3 × 0·08 mm, mounted along *b* axis, on fiber, *c* axis perpendicular to the plate; Syntex *P*Ī diffractometer with graphite monochromator; least-squares cell constants from 15 reflections (7 Friedel pairs +1) in $\sin\theta/\lambda$

range 0·34 to 0·44 Å⁻¹; systematic absences for 0*k*0, *k* odd, for *h*0*l*, *l* odd; empirical absorption correction based on *ψ* scans on 6 reflections (min. correction 0·83, max. 1·00, av. 0·94); max. 2θ 50·6°; range of *hkl* 0 to 12, 0 to 16, −13 to 13; three standard reflections, total decay −0·1%, intensities in counts with e.s.d.'s and σ(*F*²) in parentheses 7254 (44; 176), 30 083 (117; 476), 17 143 (88; 359); 1626 out of ~2850 possible quadrant data recorded by θ/2θ scans with variable scan rate (min. 4° min⁻¹, max. 24° min⁻¹), scan width above and below *K*α₁ and *K*α₂ ±0·9°, background measured for half peak time, skipping reflections below threshold (10 counts s⁻¹) on pre-scan; 73 (includes 17 systematic absences not skipped on pre-scan) measurements had *I* < 2σ(*I*), σ based on counting statistics, yielding 1462 unique observations used in least squares, after 91 pairs of symmetry-related reflections averaged; $R_{int} = 0.016$. Structure solved by combination of direct methods and difference Fourier syntheses, refined against *F*, 211 variables, including 16 anisotropic atoms and 22 H-atom *x, y, z*'s, H-atom temperature factors fixed at values of equivalent isotropic *B* of their carbon; $R_w = 0.036$, $S = 1.047$, $w = 4F^2/[\sigma^2(I) + 0.0016I^2]$; max. Δ/σ 0·39, av. Δ/σ < 0·1; max. peak in final difference map 0·32 e Å⁻³. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). All computer programs were from the Enraf–Nonius (1979) *Structure Determination Package*, run on a PDP 11/60 at Molecular Structure Corporation, College Station, TX, with procedures as indicated by Bino, Cotton & Fanwick (1979). The atomic parameters are given in Table 1 and distances and angles in Table 2.*

Discussion. The molecule is shown in stereo in Fig. 1. Some other stereo illustrations, including a packing diagram, appear in the supplementary material. The molecule is rather crowded and the structure is shown most clearly in stick form (program *PACK*; Swanson, Rosenfield & Meyer, 1982) in the supplementary material. Another *ORTEP* illustration appears in Yoon *et al.* (1983). The bonds, angles and thermal parameters are unremarkable, with thermal parameters increasing for atoms towards the ends of the ether and alkyl groupings. A few hydrogen distances and angles vary considerably from the ideal but are reported as refined, in the supplementary material.

In the crystal, the molecule gives an impression of 'neatness', probably because of the near-alignment of hydrogens on corresponding methyl groups and the

Table 1. *Coordinates and equivalent isotropic temperature factors (with e.s.d.'s)*

	x	y	z	$B_{eq}(\text{Å}^2)^*$
I	0·14006 (5)	0·15748 (3)	0·38287 (4)	4·486 (9)
O(1)	0·3954 (4)	0·4113 (3)	0·5290 (4)	4·1 (1)
O(2)	0·2461 (4)	0·6844 (3)	0·3915 (4)	4·6 (1)
N	0·2324 (5)	0·4732 (3)	0·2557 (4)	3·0 (1)
C(1)	0·2643 (6)	0·5147 (4)	0·3843 (5)	3·0 (1)
C(2)	0·2632 (6)	0·4415 (4)	0·4881 (5)	3·6 (1)
C(3)	0·2032 (7)	0·4988 (5)	0·5812 (5)	4·7 (2)
C(4)	0·1583 (7)	0·5818 (5)	0·5398 (6)	4·9 (2)
C(5)	0·1760 (6)	0·5990 (4)	0·4081 (5)	3·4 (1)
C(6)	0·4006 (8)	0·3302 (5)	0·6082 (6)	6·0 (2)
C(7)	0·1641 (8)	0·7667 (5)	0·3874 (8)	6·8 (2)
C(8)	0·0956 (6)	0·4294 (5)	0·2303 (5)	3·9 (1)
C(9)	0·2398 (6)	0·5506 (4)	0·1623 (5)	3·6 (1)
C(10)	0·3298 (6)	0·3938 (5)	0·2347 (5)	4·0 (1)
C(11)	0·4680 (6)	0·4272 (5)	0·2449 (6)	4·8 (2)
C(12)	0·5292 (8)	0·4295 (7)	0·1471 (8)	7·3 (2)

$* B_{eq} = \frac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(1,2)].$

Table 2. *Distances (Å) and angles (°)*

|			
N–C(1)	1·517 (7)	O(1)–C(2)	1·421 (7)
N–C(8)	1·513 (8)	O(1)–C(6)	1·426 (9)
N–C(9)	1·505 (7)	O(2)–C(5)	1·422 (7)
N–C(10)	1·535 (8)	O(2)–C(7)	1·423 (10)
C(1)–C(2)	1·538 (8)	C(3)–C(4)	1·306 (10)
C(1)–C(5)	1·535 (8)	C(11)–C(12)	1·329 (12)
C(2)–C(3)	1·507 (9)		
C(4)–C(5)	1·509 (9)		
C(10)–C(11)	1·477 (10)		
C(1)–N–C(8)	112·5 (5)	C(2)–O(1)–C(6)	111·9 (6)
C(1)–N–C(9)	109·6 (5)	C(5)–O(2)–C(7)	112·3 (6)
C(10)–N–C(8)	106·4 (5)		
C(10)–N–C(9)	108·3 (5)	C(2)–C(3)–C(4)	113·3 (6)
C(8)–N–C(9)	108·2 (5)	C(5)–C(4)–C(3)	112·8 (7)
C(1)–N–C(10)	111·6 (5)	C(10)–C(11)–C(12)	120·9 (8)
C(3)–C(2)–C(1)	101·7 (5)	C(4)–C(5)–C(1)	101·9 (6)
C(3)–C(2)–O(1)	114·3 (5)	C(4)–C(5)–O(2)	113·4 (5)
C(1)–C(2)–O(1)	108·4 (5)	C(1)–C(5)–O(2)	107·6 (5)
C(2)–C(1)–C(5)	108·2 (5)	C(5)–C(1)–N	114·4 (5)
C(2)–C(1)–N	114·4 (5)	C(11)–C(10)–N	113·3 (6)
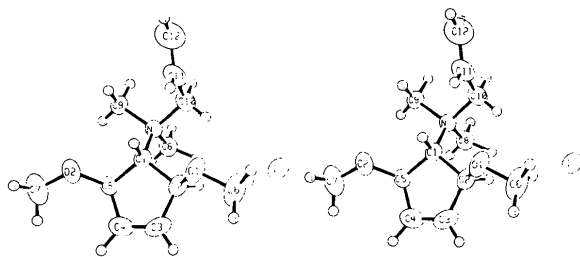
Fig. 1. Stereoview of an individual molecule with 50% probability thermal ellipsoids. Hydrogens have arbitrary radius. Within the hydrogen spheres, single dots, double dots and no dots indicate hydrogens *A, B, C.*

near-parallel or near-perpendicular arrangement of various planes of atoms. For example, the atoms I, N, C(8), H(8*B*), C(1) and H(1) lie in a plane that perpendicularly slices the ring. They are coplanar to within 0·07 (3) Å [C(1)]. The 'allyl plane' [C(10) to C(12) plus hydrogens] is also parallel to this 'slicing plane' [dihedral angle 9 (1)° with plane of C(1), N, C(8)], and perpendicular [96 (1)°] to the mean ring plane C(1) to C(5), planar to within 0·09 (3) Å [C(1)]. The nitrogen is 1·31 (3) Å out of the allyl plane, and the iodine is 2·04 (3) Å out of the ring, C(1) is 0·23 (3) Å out of the C(2) to C(5) plane, on the same side as the oxygens, which are 0·97 (3) Å out of the mean ring plane. The nitrogen is 0·78 (3) Å out on the opposite side, and C(8) is 2·26 (3) Å out. [C(6) and C(7), the ether methyls, are 0·74 (3), 0·77 (3) Å out.] Double-bonded ring carbons C(3) and C(4) are 0·35 (3) Å out of the plane of C(1), C(2), C(5). The dihedral angle of the ring 'envelope' is 15 (1)° [C(1) is the tip of the flap].

One hydrogen on each nitrogen methyl and one on C(12) appear to point toward the iodide ion (supplementary figures). They are within 3·2 (1) Å of it. H to I distances less than 4 Å are given in the supplementary material.

This compound is the product of a light-triggered reaction starting from a nitrogen-containing six-membered ring. The nitrogen has been extruded from the ring, and two methoxy groups picked up from the solvent. The interesting photochemistry is discussed in the Yoon *et al.* (1982, 1983) references.

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