Table VI B
Bond Angles (in deg) in five member rings in $C_{26}H_{25}NO$
With Estimated Standard Deviations

C (1) – C (2) – C (3)	111.5 (6)
C (2) – C (3) – C (8)	115.2 (6)
C (3) – C (8) – N (4)	107.9 (5)
C (8) – N (4) – C (5)	105.4 (5)
N (4) – C (5) – C (6)	105.2 (6)
C (5) – C (6) – C (7)	102.2 (6)
C (6) – C (7) – C (8)	104.4 (5)
C (6) – C (7) – C (1)	114.9 (5)
C (8) – C (7) – C (1)	106.2 (5)
C (7) – C (1) – C (2)	103.6 (5)
C (7) – C (8) – C (3)	103.4 (5)
C (7) – C (8) – N (4)	106.3 (5)
C (9) – C (6) – C (7)	111.4 (6)
C (9) – C (6) – C (5)	112.2 (6)
O – C (1) – C (7)	108.8 (5)
O – C (1) – C(21)	111.6 (5)
C (2) – C (1) – C (21)	112.2 (5)
C (1) – C (2) – C (11)	122.6 (6)
C (3) – C (2) – C (11)	125.7 (6)
C (3) – C (8) – C (31)	113.0 (6)
N (4) – C (8) – C (31)	109.0 (5)
C (1) – O – H (0)	114
C (2) – C (3) – H (3)	123
C (8) – C (3) – H (3)	120
C (8) – N (4) – H (4)	100
C (5) – N (4) – H (4)	112
N (4) – C (5) – H (51)	106
N (4) – C (5) – H (52)	110
C (6) – C (5) – H (51)	111
C (6) – C (5) – H (52)	110
H (51) – C (5) – H (52)	114
C (5) – C (6) – H (6)	112
C (7) – C (6) – H (6)	109
C (9) – C (6) – H (6)	110
C (1) – C (7) – H (7)	116
C (6) – C (7) – H (7)	112
C (8) – C (7) – H (7)	101
H (91) – C (9) – H (92)	97
H (91) – C (9) – H (93)	82
H (92) – C (9) – H (93)	107

Table VII
Dihedral Angles for Various Planes in $C_{26}H_{25}NO$*

Plane A	Plane B	Angle (deg)
1	2	89.9
1	3	57.7
1	4	26.8
1	5	79.1
2	3	34.2
2	4	82.5
2	5	11.2
3	4	73.1
3	5	45.3
4	5	73.4

*Plane 1. Plane Through C_{11}–C_{16}
Plane 2. Plane Through C_{21}–C26
Plane 3. Plane Through C_{31}–C_{36}
Plane 4. Plane Through C_1, C_2, C_3, C_7, C_8
Plane 5. Plane Through N_4, C_5, C_6, C_7, C_8

References

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Table V A
Bond Distances (in A°) in Phenyl Rings in $C_{26}H_{25}NO$
With Estimated Standard Deviations

	n = 1	n = 2	n = 3
C (n1) – C (n2)	1.410 (11)	1.400 (12)	1.334 (11)
C (n2) – C (n3)	1.376 (10)	1.412 (14)	1.408 (14)
C (n3) – C (n4)	1.377 (14)	1.349 (16)	1.276 (16)
C (n4) – C (n5)	1.380 (13)	1.411 (18)	1.390 (14)
C (n5) – C (n6)	1.390 (10)	1.356 (11)	1.364 (13)
C (n6) – C (n1)	1.387 (11)	1.384 (10)	1.412 (13)
C (n2) – H (n2)	1.06	1.28	1.14
C (n3) – H (n3)	1.22	1.02	1.07
C (n4) – H (n4)	1.16	1.05	0.89
C (n5) – H (n5)	0.97	1.04	1.20
C (n6) – H (n6)	1.15	1.04	1.09

Table V B
Bond Distances (in A°) in five member rings in $C_{26}H_{25}NO$
With Estimated Standard Deviations

C (1) – C (2)	1.521 (10)
C (2) – C (3)	1.321 (10)
C (3) – C (8)	1.488 (9)
C (8) – N (4)	1.502 (8)
N (4) – C (5)	1.463 (11)
C (5) – C (6)	1.527 (11)
C (6) – C (7)	1.526 (9)
C (7) – C (8)	1.566 (11)
C (7) – C (1)	1.577 (9)
C (1) – 0	1.415 (8)
C (1) – C (21)	1.554 (9)
C (2) – C (11)	1.496 (8)
C (8) – C (31)	1.532 (10)
C (6) – C (9)	1.503 (10)
O – H (0)	0.96
C (3) – H (3)	0.92
N (4) – H (4)	1.07
C (5) – H (51)	1.08
C (5) – H (52)	0.92
C (6) – H (6)	1.10
C (7) – H (7)	1.02
C (9) – H (91)	1.02
C (9) – H (92)	1.00
C (9) – H (93)	0.83

Table VI A
Bond Angles (in deg) in Phenyl Rings in $C_{26}H_{25}NO$
With Estimated Standard Deviations

	n = 1	n = 2	n = 3
C (n1) – C (n2) – C (n3)	120.8 (7)	118.2 (8)	123.0 (9)
C (n2) – C (n3) –C (n4)	119.8 (8)	121.9 (10)	119.3 (11)
C (n3) – C (n4) – C (n5)	120.7 (8)	119.1 (10)	122.1 (11)
C (n4) – C (n5) – C (n6)	119.7 (8)	119.9 (9)	118.4 (10)
C (n5) – C (n6) – C (n1)	120.7 (7)	121.6 (7)	121.4 (9)
C (n6) – C (n1) – C (n2)	118.3 (6)	119.3 (7)	115.9 (8)
C (n1) – C (n2) – H (n2)	119	116	120
C (n3) – C (n2) – H (n2)	121	126	114
C (n2) – C (n3) – H(n3)	113	122	101
C (n4) – C (n3) – H (n3)	127	115	132
C (n3) – C (n4) – H (n4)	126	135	114
C (n5) – C (n4) – H (n4)	113	106	123
C (n4) – C (n5) – H (n5)	106	107	110
C (n6) – C (n5) – H (n5)	130	132	119
C (n5) – C (n6) – H (n6)	120	123	117
C (n1) – C (n6) – H (n6)	119	115	121

Table III

Final Thermal Parameters ($x10^{+4}$) For $C_{26}H_{25}NO$ The Form of the thermal parameter is

$$\exp[-2\pi^2(u_{11}h^2a^{*2}+u_{22}K^2b^{*2}+u_{33}l^2c^{*2}+2u_{12}hKa^*b^*+2u_{13}hla^*c^*+2u_{23}Klb^*c^*)]$$

ATOM	U11	U22	U33	U12	U13	U23
0	52 (2)	49 (3)	54 (3)	− 12 (2)	1 (2)	12 (2)
N (4)	46 (3)	49 (3)	44 (4)	7 (2)	5 (2)	2 (2)
C (1)	45 (3)	35 (3)	38 (4)	− 2 (2)	− 3 (2)	2 (2)
C (2)	40 (3)	46 (4)	30 (4)	− 4 (3)	5 (2)	− 1 (3)
C (3)	40 (3)	39 (3)	36 (4)	− 3 (2)	0 (2)	− 8 (3)
C (5)	45 (4)	64 (4)	53 (5)	− 4 (3)	8 (3)	6 (4)
C (6)	40 (3)	51 (4)	57 (4)	0 (3)	− 2 (3)	− 1 (3)
C (7)	42 (3)	34 (3)	38 (4)	− 1 (2)	− 4 (2)	2 (3)
C (8)	39 (3)	38 (3)	42 (4)	0 (3)	2 (3)	0 (3)
C (9)	45 (4)	94 (6)	95 (6)	− 12 (4)	− 23 (4)	− 11 (5)
C (11)	42 (3)	50 (4)	41 (4)	− 12 (3)	2 (3)	6 (3)
C (12)	60 (4)	65 (5)	44 (4)	− 7 (4)	− 11 (3)	3 (4)
C (13)	69 (4)	94 (6)	49 (5)	− 12 (4)	− 19 (3)	− 6 (4)
C (14)	49 (4)	99 (7)	61 (5)	− 7 (5)	− 14 (3)	17 (5)
C (15)	37 (4)	90 (6)	65 (5)	3 (4)	− 2 (3)	22 (5)
C (16)	38 (3)	61 (5)	45 (4)	0 (3)	0 (3)	3 (3)
C (21)	50 (4)	55 (4)	44 (4)	5 (3)	− 8 (3)	− 4 (3)
C (22)	72 (6)	53 (4)	80 (6)	12 (4)	− 16 (4)	− 26 (4)
C (23)	97 (7)	74 (6)	114 (7)	29 (5)	− 20 (6)	− 46 (6)
C (24)	69 (6)	134 (10)	90 (7)	20 (6)	− 5 (5)	− 46 (6)
C (25)	52 (4)	143 (9)	52 (5)	18 (5)	6 (4)	− 15 (5)
C (26)	54 (4)	73 (5)	48 (4)	− 1 (4)	4 (3)	− 9 (4)
C (31)	54 (4)	47 (5)	42 (5)	− 4 (3)	− 1 (3)	3 (3)
C (32)	142 (8)	65 (6)	66 (6)	6 (5)	31 (5)	10 (5)
C (33)	213 (10)	70 (5)	62 (6)	29 (6)	36 (6)	1 (5)
C (34)	228 (10)	69 (8)	56 (5)	− 7 (7)	5 (5)	29 (5)
C (35)	177 (11)	65 (6)	75 (6)	13 (6)	6 (6)	13 (5)
C (36)	133 (8)	59 (5)	60 (6)	15 (5)	17 (5)	7 (4)

Table IV

Final Hydrogen Atom Parameters ($x10^{+3}$) For $C_{26}H_{25}NO$ and B is the isotropic thermal parameter.

ATOM	X	Y	Z	
H (0)	590 (0)	410 (0)	988 (0)	4.0 (0.0)
H (3)	649 (0)	824 (0)	968 (0)	4.0 (0.0)
H (4)	278 (0)	844 (0)	918 (0)	4.0 (0.0)
H (6)	286 (0)	496 (0)	934 (0)	4.0 (0.0)
H (7)	448 (0)	623 (0)	845 (0)	4.0 (0.0)
H (12)	761 (0)	771 (0)	1056 (0)	4.0 (0.0)
H (13)	956 (0)	744 (0)	1132 (0)	4.0 (0.0)
H (14)	1128 (0)	529 (0)	1114 (0)	4.0 (0.0)
H (15)	1085 (0)	425 (0)	1033 (0)	4.0 (0.0)
H (16)	850 (0)	433 (0)	957 (0)	4.0 (0.0)
H (22)	555 (0)	300 (0)	893 (0)	4.0 (0.0)
H (23)	711 (0)	214 (0)	794 (0)	4.0 (0.0)
H (24)	903 (0)	347 (0)	738 (0)	4.0 (0.0)
H (25)	939 (0)	525 (0)	761 (0)	4.0 (0.0)
H (26)	781 (0)	641 (0)	846 (0)	4.0 (0.0)
H (32)	614 (0)	736 (0)	792 (0)	4.0 (0.0)
H (33)	648 (0)	873 (0)	725 (0)	4.0 (0.0)
H (34)	518 (0)	1071 (0)	728 (0)	4.0 (0.0)
H (35)	354 (0)	1130 (0)	810 (0)	4.0 (0.0)
H (36)	386 (0)	1003 (0)	906 (0)	4.0 (0.0)
H (51)	350 (0)	652 (0)	1012 (0)	4.0 (0.0)
H (52)	181 (0)	695 (0)	984 (0)	4.0 (0.0)
H (92)	175 (0)	707 (0)	863 (0)	4.0 (0.0)
H (93)	131 (0)	584 (0)	840 (0)	4.0 (0.0)
H (91)	62 (0)	614 (0)	887 (0)	4.0 (0.0)

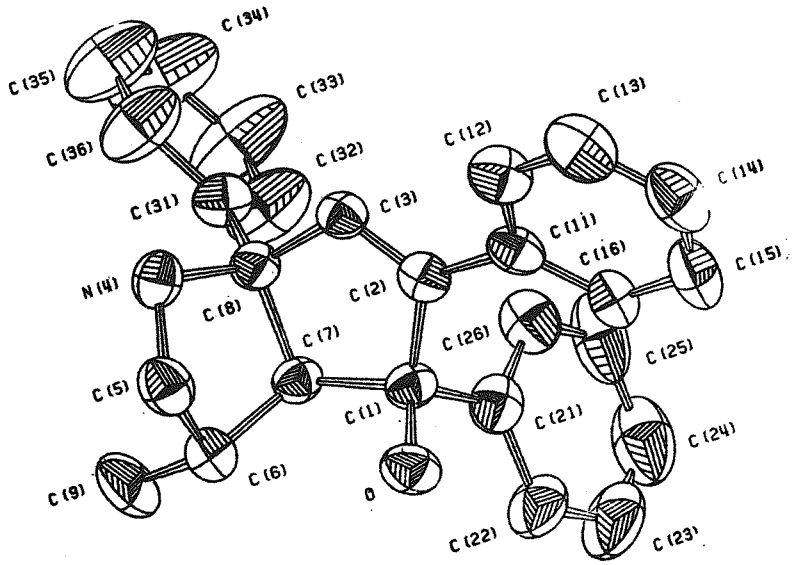

Figure 2. An ORTEP View of $C_{26}H_{25}NO$ showing the atomic numbering and the thermal ellipsoids (50% probability level).

Table I
Crystal Data for $C_{26}H_{25}NO$

Formula	*$C_{26}H_{25}NO$*
Molecular Weight	367.50
Space Group	$Pn2_1a$
a, A°	8.874 (2)
b, A°	10.793 (4)
c, A°	21.560 (6)
α, deg	90*
β, deg	90*
γ, deg	90*
Volume, A°3	2065 (1)
Z	4
Dm, g Cm^{-3}	1.175
Dc, g Cm^{-3}	1.182
Crystal Size, mm	0.32x0.20x0.25
μ, Cm^{-1}	0.662
Radiation Used	MoK_α – graphite monochromator
2 θ Range	0 – 45°
No of Measured Reflections	1444
No of Reliable Reflections	1212
K[in $I_\alpha \langle K\sigma(I)$]	2.0
Goodness of Fit	0.336
R	5.5

* Required by symmetry of space group.

Table II
Final Positional Parameters ($x10^{+4}$) For $C_{26}H_{25}NO$

ATOM	X	Y	Z
0	5165(5)	4554	9646(2)
N(4)	3483(6)	7978(7)	9506(2)
C(1)	5792(7)	5436(7)	9234(3)
C(2)	6693(7)	6415(7)	9579(2)
C(3)	6154(7)	7538(7)	9479(3)
C(5)	2811(8)	6825(8)	9732(3)
C(6)	2907(7)	5926(8)	9187(3)
C(7)	4471(6)	6197(7)	8927(3)
C(8)	4763(7)	7588(7)	9094(3)
C(9)	1702(8)	6164(10)	8711(4)
C(11)	7960(7)	6098(8)	10009(3)
C(12)	8272(8)	6901(9)	10509(3)
C(13)	9418(9)	6644(10)	10919(3)
C(14)	10248(9)	5574(10)	10851(4)
C(15)	9953(8)	4761(10)	10372(3)
C(16)	8815(7)	5029(8)	9950(3)
C(21)	6727(7)	4803(7)	8714(3)
C(22)	6511(10)	3542(8)	8591(4)
C(23)	7362(13)	2996(10)	8110(5)
C(24)	8322(11)	3663(13)	7758(5)
C(25)	8515(9)	4935(11)	7886(4)
C(26)	7740(8)	5470(9)	8357(3)
C(31)	4884(7)	8495(8)	8550(3)
C(32)	5424(13)	8221(10)	7990(4)
C(33)	5564(15)	9104(10)	7512(4)
C(34)	5127(14)	10213(11)	7608(4)
C(35)	4553(15)	10592(9)	8177(4)
C(36)	4435(12)	9737(9)	8644(4)

Crystal and Molecular Structure of 6-Hydroxy-4-Methyl-1,6,7-Triphenylazabicyclo [3,3,0] Oct-7-Ene.

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ABSTRACT

Crystal and Molecular Structure of 6-Hydroxy-4-Methyl-1,6,7-Triphenylazabicyclo (3,3,0) Oct-7-Ene, $C_{26}H_{25}NO$, was determined by X-ray diffrection. This compound crystallizes in the orthorhombic space group $Pn2_1a$ with four molecules per unit cell, all with dimensions of a=8.875(2) A^o, b=10.793(4) A^o and c=21.560(6) A^o. A total of 1444 reflections were measured and 1212 were used in the analysis. The final R value was 0.055.

We recently considered products which formed by rearrangements of N-Vinyl pyridinium pseudobases[1]. Crystal and Molecular structure of 6-Hydroxy-4-Methyl-1,6,7-Triphenylazabicyclo [3,3,0] Oct-7-Ene. has been determined by X-ray diffraction. All intensity measurements were carried out using a P1 diffractometer and Zr-filtered Mok$_\alpha$ radiation to a limit of 45°. Only reflections with $I \geq 2\sigma(I)$ were considered reliable and were used in the analysis. This structure was solved using MULTAN-78[2] and refined by least square methods. A total of 1444 reflections were measured and 1212 were used in the analysis. The final R value was 0.055 and the R value is defined as $R = \Sigma \mid F_{obs} - F_{calc} \mid / \Sigma \mid F_{obs} \mid$ The scattering factors were taken from the usual sources.[3] The crystal data is given in Table I. The final positional parameters and thermal parameters for non-hydrogen atoms are given in Tables II and III respectively. The hydrogen atom parameters, bond distances, and bond angles are given in Tables IV, V, and VI respectively.

The distances and angles are not unusual. There is a C – C double bond between C(2) – C(3) [1.321 (10) A^o]. The dihedral angles for various planes is given in Table VII. The least-squares planes data show the deviations of atoms from planarity are from-0.009 to 0.006 A^o in plane 1, from-0.010 to 0.014 A^o in plane 2,from -0.007 to 0.009 A^o in plane 3,from -0.015 to 0.023 A^o in plane 4 and from –0.220 to 0.248 A^o in plane 5. The dihedral angle between the two five-membered rings is 73.4°. Stereoscopic view of $C_{26}H_{25}NO$ is given in Figure 1. Figure 2 shows an ORTEP view of $C_{26}H_{25}NO$ with the atomic numbering and the thermal ellipsoids (50% probability level).

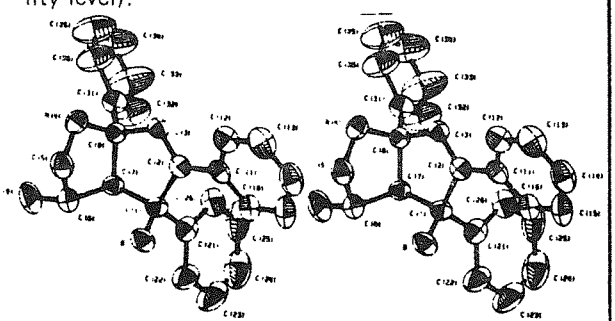

Figure 1. Stereoscopic view of $C_{26}H_{25}NO$