$C(5\alpha)$ — $C(5)$ — $C(4)$	129.1 (4)	$C(5\beta) - C(5\alpha) - C(5)$	113.6 (4)
$O(5\gamma) - C(5\beta) - C(5\alpha)$	113.3 (4)	C(3,5') - N(3) - C(2)	120.0 (3)
C(3,5')N(3)C(4)	123.9 (4)	N(3') - C(2') - N(1')	126.3 (4)
C(4') - N(3') - C(2')	117.8 (4)	C(4') - C(5') - C(3,5')	121.0 (4)
C(5') - C(3,5') - N(3)	112.0 (4)	C(5') - C(4') - N(3')	120.5 (4)
C(5') - C(6') - N(1')	124.1 (4)	C(6') - N(1') - C(2')	115.6 (4)
C(6') - C(5') - C(3,5')	123.1 (4)	C(6') - C(5') - C(4')	115.7 (4)
$C(2'\alpha) - C(2') - N(1')$	116.5 (4)	$C(2'\alpha) - C(2') - N(3')$	117.2 (4)
$N(4'\alpha) - C(4') - N(3')$	117.2 (4)	$N(4'\alpha) - C(4') - C(5')$	122.3 (4)
C(1A) - C(2A) - C(3A)	122. (2)	O(A) - C(2A) - C(1A)	118 (2)
O(A) - C(2A) - C(3A)	120 (2)		

Table 3. Hydrogen-bonding geometry (Å, °)

D — $H \cdot \cdot \cdot A$	H <i>A</i>	$D \cdots A$	$D = H \cdots A$
$N(4'\alpha) - H(1) \cdots O(5\gamma^{i})$	1.97 (5)	2.915 (5)	173 (5)
$N(4'\alpha) \rightarrow H(2) \cdots N(3'^{ii})$	2.26 (5)	3.117 (5)	165 (5)
$O(5\gamma)$ -H···N(1 ^{'iii})	1.95 (5)	2.814 (4)	176 (5)
Symmetry codes: (i) -	$x, \frac{1}{2} + y, \frac{1}{2} - (iii) - x, 1 - y$	z; (ii) $1 - xz, 1 - z.$, 2 - y, 1 - z;

The structure was solved by direct methods and refined by full-matrix least squares using *SHELX*76 (Sheldrick, 1976). A difference map after anisotropic refinement of the TTT molecule revealed the peaks for all H atoms of TTT and additional prominent peaks near the inversion centre at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. These peaks were identified, with difficulty, as the disordered acetone solvate, based on the interpretation of the geometrical relationships of the peaks, the NMR spectra and the elemental analysis data of the crystal. In the final cycle of refinement, each H atom was assigned a fixed isotropic displacement parameter 1.3 times greater than the isotropic equivalent of the atom to which it is attached. H atoms in the acetone molecule could not be located and were not included in the structure-factor calculations.

This work was supported by a grant from the Korea Science and Engineering Foundation.

Lists of structure factors, anisotropic displacement parameters, Hatom coordinates and bond distances and angles involving H atoms have been deposited with the IUCr (Reference: HR1001). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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The Novel GABA_A Receptor Ligand NNC 14-0764: 5-(3-Cyclopropyl-1,2,4-oxadiazol-5-yl)-2,3-dihydrodiimidazo[1,5-*a*:1',2'-*c*]-quinazoline

REX A. PALMER,* ROBERT W. JANES AND ADAM L. CORPER

Department of Crystallography, Birbeck College, Malet Street, London WC1E 7HX, England

JOHN N. LISGARTEN

Department of Ultrastructure, Instituut voor Moleculaire Biologie, Vrije Universiteit Brussel, Paardenstraat 65, B-1640 Sint-Genesius-Rode, Belgium

HOLGER C. HANSEN

CNS Division, Novo Nordisk A/S, Novo Nordisk Park, 2760 Maaloev, Denmark

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Abstract

The crystal and molecular structure of the title compound, $C_{17}H_{14}N_6O$, has been determined. The two molecules in the asymmetric unit have very similar geometrical features, the major difference being in the overall convex or concave shape of the molecular surface. As a consequence, although as expected, the cyclopropyl rings are approximately perpendicular to the general molecular plane; the three C atoms of the cyclopropyl groups are distributed quite differently above and below the general molecular plane in the two molecules. Consequences of this effect for theoretical consideration of drug activity are discussed.

Comment

The title compound (Ia) is a member of a novel series of compounds which exhibit strong affinity for the GABA_A receptor (Im, Im, Pregenzer, Petke, Hamilton, Carter, von Voigtlander, Hansen & Kristiansen, 1992). These drugs act upon the central nervous system, and although they are similar in chemical structure they have remarkably different pharmacological properties (Im *et al.*, 1992). The objectives of the present study were to confirm the molecular structure of (Ia) and to provide accurate geometrical parameters for future quantitative structure–activity studies of these compounds.



Fig. 1 shows a view of molecule 1 perpendicular to the least-squares plane and the numbering scheme used in the X-ray analysis. The assignment of the atom labels C2B and C3B in the cyclopropyl rings of the two molecules is arbitrary, and the actual choice of labelling has been made in order to maximize compatibility between the descriptions of molecular geometry given below.

The bond lengths for the two molecules in the asymmetric unit agree within acceptable limits, and confirm, essentially, the assigned structure of (Ia). Of the small variations in the lengths of bonds of the same type observed in these two structures, the most significant are for the N=C bonds N1=C16, N7=C8, N1A=C5A and N4A=C3A, with values ranging from 1.274 (2) to 1.301 (2) Å, the larger values being for the linked oxadiazole ring A (Fig. 1) external to the fused heterocyclic ring system CDEF. There are no unusual bond angles. Significant variations in the external ring angles of the two molecules are noted in Fig. 1 and in Table 2; the torsion angles in the two molecules are very similar. The differences



Fig. 1. A view of molecule 1 perpendicular to the least-squares plane, showing the atom-numbering scheme used in the X-ray analysis (atom numbers in molecule 1 are primed). An asterisk (*) denotes external ring angles differing by $>3\sigma$ between molecules 1 and 2.

in conformation can be illustrated by comparing the dihedral angles in different parts of the two molecules. In both molecules, the diimidazoguinazoline moieties (rings C, D, E and F) and the oxadiazole rings (A) are essentially planar. The equations for the relevant least-squares planes and the deviations of atom positions from them are given in Table 3. From these data it can be seen that the dihedral angles between the cyclopropyl ring B and the oxadiazole ring A differ by about $3.7 (2)^{\circ}$ between molecules 1 and 2 but with atom C2B above, C3B below and C1 B lying approximately in the oxadiazole ring plane in both molecules. As a consequence of differences between the diimidazoquinazoline plane and oxadiazole plane in the two molecules, however, atom C2B is above, C3B below and C1B lies approximately in the plane of the diimidazoquinazoline group in molecule 1, whereas in molecule 2, atoms C1B' and C3B' are both below and C2B' lies approximately in this plane. The consequences of these differences in molecular conformation can be seen in Fig. 2, which indicates a dramatic overall difference in the curvature of the two molecules.



Fig. 2. Molecular profiles showing the opposing curvature of the two molecules in the asymmetric unit, where the atoms labelled *B* are part of the cyclopropyl rings.



Fig. 3. A view of the crystal packing showing the stacking of the ring systems.

The molecules form van der Waals stacks (Fig. 3) in the crystal structure, there being no other types of intermolecular forces present.

Previous studies (Im et al., 1992) indicated that the energetics of analogues in the present series of diimidazoquinazolines are based on the relative orientations of the cyclopropyloxadiazole group and the diimidazoquinazoline ring system treated as two separate units. The present analysis fortuitously affords two independent conformers of one member of the series, and suggests that in view of the differences observed in the orientation of the cyclopropyl group the approach should in fact proceed via consideration of the cyclopropyl group, the oxadiazole ring and the diimidazoquinazoline group, and their relative orientations.

Experimental Crystal data

~	
C ₁₇ H ₁₄ N ₆ O	Cu $K\alpha$ radiation
$M_r = 318.34$	$\lambda = 1.54178 \text{ Å}$
Monoclinic	Cell parameters from 25
$P2_1/a$	reflections
a = 8.693 (3) Å	$\theta = 20-25^{\circ}$
b = 26.794 (7) Å	$\mu = 0.790 \text{ mm}^{-1}$
c = 12.534 (5) Å	T = 293 K
$\beta = 93.08$ (3)°	Needle
$V = 2915.0 \text{ Å}^3$	$0.6 \times 0.3 \times 0.3$ mm
Z = 8	Colourless
$D_{\rm x} = 1.451 {\rm Mg m}^{-3}$	Crystal source: Novo
	Nordisk

Data collection	
Enraf–Nonius CAD-4	$\theta_{\rm max} = 73^{\circ}$
diffractometer	$h = -10 \rightarrow 9$
ω –2 θ scans	$k = -15 \rightarrow 33$
Absorption correction:	$l = -15 \rightarrow 15$
none	3 standard reflections
11 733 measured reflections	monitored every 10
5833 independent reflections	reflections
5149 observed reflections	intensity decay:
$[I > 2\sigma(I)]$	<10%
$R_{\rm int} = 0.0287$	

100

Refinement

Refinement on F^2 $\Delta \rho_{\rm max} = 0.213 \ {\rm e} \ {\rm \AA}^{-3}$ $\Delta \rho_{\rm min} = -0.186 \ {\rm e} \ {\rm \AA}^{-3}$ $R[I > 2\sigma(I)] = 0.0365$ $wR(F^2) = 0.1053$ Extinction correction: SHELXL92 (Sheldrick, S = 1.0005833 reflections 1992) Extinction coefficient: 0.002 462 parameters Only H-atom U's refined (1) $w = 1/\sigma^2(F_o^2)$ Atomic scattering factors $(\Delta/\sigma)_{\rm max} = -0.001$ (for the from SHELXL92 z coordinate of N9) (Sheldrick, 1992)

Fable	1. Fractional	atomic c	oordinates	and	equival	ent
	isotropic dis	placemen	t paramete	ers (Å	²)	

	⊂eq -	- (1/3)2;250;50	<i>i uj uruj</i> .	
	, <i>x</i>	у	z	U_{eq}
Molecule	1	0 (073 (1)	0 5022 (1)	0.055 (1)
NI	0.5819(2)	0.6072(1)	0.3922 (1)	0.053(1)
C2	0.6491 (2)	0.6235(1)	0.4927(1)	0.033(1)
C3	0.7407 (2)	0.5793(1)	0.4512(1)	0.048 (1)
N4	0.6870(1)	0.5390(1)	0.5186(1)	0.044 (1)
C5	0.7352 (2)	0.4904 (1)	0.5211 (1)	0.041 (1)
C6	0.8247 (2)	0.4603(1)	0.4598 (1)	0.044 (1)
N7	0.8311 (2)	0.4125(1)	0.5038(1)	0.051 (1)
C8	0.7495 (2)	0.4139(1)	0.5867 (1)	0.050(1)
N9	0.6874 (2)	0.4606(1)	0.6025(1)	0.044 (1)
C10	0.5983 (1)	0.4777 (1)	0.6858(1)	0.044 (1)
C11	0.5566 (2)	0.4462 (1)	0.7670(1)	0.052(1)
C12	0.4745 (2)	0.4650(1)	0.8490(1)	0.058 (1)
C13	0.4314 (2)	0.5148 (1)	0.8493 (1)	0.061 (1)
C14	0.4704 (2)	0.5462 (1)	0.7681 (1)	0.054 (1)
C15	0.5558 (2)	0.5280(1)	0.6856(1)	0.045 (1)
C16	0.6054(2)	0.5603 (1)	0.6002(1)	0.044 (1)
N1A	1.0633 (2)	0.4509(1)	0.2388 (1)	0.061 (1)
O2A	0.9935(1)	0.4329(1)	0.3315(1)	0.059 (1)
C3A	0.9056 (2)	0.4701 (1)	0.3652(1)	0.043 (1)
N4A	0.9109(1)	0.5098 (1)	0.3056(1)	0.049 (1)
C5A	1.0091 (2)	0.4959(1)	0.2287 (1)	0.047 (1)
C1 <i>B</i>	1.0532 (2)	0.5290(1)	0.1426 (1)	0.056 (1)
C2B	1.0571 (2)	0.5839(1)	0.1627 (2)	0.065 (1)
C3B	0.9358 (2)	0.5628 (1)	0.0895 (2)	0.073 (1)
Molecule	2			
N1'	0.7234 (2)	0.3444 (1)	0.1735(1)	0.054 (1)
C2′	0.8064 (2)	0.3625(1)	0.0825(1)	0.058 (1)
C3′	0.8706 (2)	0.3167(1)	0.0257 (1)	0.048 (1)
N4'	0.8070(1)	0.2761 (1)	0.0873 (1)	0.045(1)
C5′	0.8265 (2)	0.2258(1)	0.0751(1)	0.042(1)
C6'	0.8988(1)	0.1947(1)	0.0055(1)	0.045(1)
N7'	0.8770(2)	0.1451(1)	0.0353(1)	0.054 (1)
C8'	0.7965(1)	0.1466(1)	0.1184 (1)	0.053 (1)
N9'	0.7606 (1)	0.1949(1)	0.1474 (1)	0.045 (1)
C10'	0.6706 (2)	0.2118(1)	0.2304 (1)	0.044 (1)
ČŮľ	0.5977(1)	0.1785(1)	0.2956 (1)	0.054 (1)
C12'	0.5081 (2)	0.1966(1)	0.3742(1)	0.060(1)
C13'	0.4940 (2)	0.2475(1)	0.3901 (1)	0.061(1)
C14'	0.5666 (2)	0.2809(1)	0.3253(1)	0.055(1)
		/	/	

$U_{aa} = (1/3) \sum_i \sum_j U_{ij} a^* a^* a_i a_j$

PALMER, JANES, CORPER, LISGARTEN AND HANSEN

C15′ 0.6543 (2)	0.2632	(1) 0.2438 (1)	0.045(1)	N1A-C5A-N4A	114.7 (1)	N1A'-C5A'		115.0(1)
$U_{10} = 0.7274(1)$	0.2969	(1) 0.1/06(1) 0.2272(1)	0.044(1)	NIA - C5A - C1B	121.8(1)	NIA'	-ClB'*	123.1 (1)
02A' 1.0424 (1)	0.1655	=0.2272(1) =0.1370(1)	0.003(1) 0.059(1)	C5A = C1B = C2B	123.5(1) 118 5(1)	$C5A' \rightarrow C1B'$	-C3B'	121.9(1)
C3A' = 0.9830(2)	0.2050	(1) = -0.0871(1)	0.035(1)	$C5A \rightarrow C1B \rightarrow C2B$	110.5(1)	C5A' - C1B'		1177(2)
N4A' 1.0102 (2)	0.2471	(1) -0.1341(1)	0.051 (1)	C2B - C1B - C3B	59.1 (1)	C3B' - C1B'	-C2B'	58.9 (1)
C5A' 1.0915 (2)	0.2327	(1) -0.2198(1)	0.053(1)	C3B-C2B-C1B	60.5 (1)	C3B'C2B'	C1 <i>B</i> ′	60.6 (1)
C1B' 1.1451 (2)	0.2688	-0.2970(2)	0.065(1)	C2B—C3B—C1B	60.3 (1)	C2B'-C3B'	—C1 <i>B</i> ′	60.7 (1)
C2B' 1.1857 (2)	0.3203	(1) -0.2581(1)	0.068(1)	C5C6	-C3AN4A		-47(2)	
C3B' 1.0427 (2)	0.3126	-0.3249(1)	0.066(1)	N7	-C3A—N4A		175.3 (1)	
T-1-1- 2 C-1			Å 0.5	C5C6	-C3AO2A		174.2 (1)	
Table 2. Sel	ectea geon	ietric parameters (A, ⁻)	N7—C6—	-C3A—O2A		-5.8 (2)	
N1-C16	1.275 (2)	N1'-C16'	1.274 (2)	N1A	4—C1 <i>B</i> —C2 <i>B</i>		-149.3 (1)	
N1C2	1.470 (2)	N1'-C2'	1.465 (2)	N4A	A - C1B - C2B		29.4 (2)	
C2—C3	1.532 (2)	C2′—C3′	1.537 (2)	NIA-CS/	A = C1B = C3B		141.9(1)	
C3—N4	1.467 (1)	C3'N4'	1.461 (1)	N4A			-39.4(2)	
N4-C3	1.300(1)	N4 - C3 N4' - C16'	1.300(1)	C5A-C1/	$B \rightarrow C3B \rightarrow C2B$		107.4(1)	
C5-N9	1.378 (1)	C5' - N9'	1.375(1)	C5'-C6'	-C3A'-N4A'*		-2.8(2)	
C5-C6	1.383 (2)	C5' - C6'	1.383 (2)	N7'—C6'	-C3A'-N4A'		175.4 (1)	
C6N7	1.396 (1)	C6'N7'	1.397 (1)	C5'—C6'	-C3A'-O2A'*		178.8 (1)	
C6—C3A	1.435 (2)	C6'-C3A'	1.432 (2)	N7′—C6′			-3.0 (2)	
N7—C8	1.290 (2)	N7′—C8′	1.286 (2)	NIA'-C	A' - CIB' - C3B'	3' n/*	149.3 (2)	
C8—N9	1.383 (2)	C8'	1.386 (2)	N4A	A = CIB = C3L A' = CIB' = C3L	5 * 2'*	-1431(3)	
N9-CIU	1.408(1)	N9 - C10	1.409 (2)	N44'-C'	A' = C1B' = C2B'	, ?′∗	-363(2)	
C10C15	1.308 (2)	C10' - C15'	1.380 (2)	C5A'-C1	B' - C2B' - C3B	3′	-107.1(2)	
C11-C12	1.378 (2)	C10' - C12'	1.376(2)	C5A'-C1	B'-C3B'-C2E	3′*	107.7 (2)	
C12-C13	1.387 (2)	C12'-C13'	1.384 (2)					
C13—C14	1.377 (2)	C13'—C14'	1.383 (2)	* Denotes a para	meter which d	iffers significa	ntly in valu	ie between
C14C15	1.394 (2)	C14'-C15'	1.391 (2)	molecules 1 and 2.				
C15—C16	1.459 (2)	C15'-C16'	1.457 (2)	Tabl	2 Loget of	waraa nlan	on data	
NIA-CSA	1.297 (2)	NIA' = C5A' NIA' = O2A'	1.299 (2)	Table	z 5. Leusi-sq	iuures-piune	es uala	
$\Omega^2 A \rightarrow C^3 A$	1.425(1) 1 340(1)	02A' - C3A'	1.420(2) 1.347(1)	Molecule 1, diimida	zoquinazoline	group		
C3A—N4A	1.301 (2)	C3A'-N4A'	1.298 (2)		-	-		
N4A—C5A	1.373 (2)	N4A'-C5A'	1.372 (2)	Equation of plane: 7.02	23(1)x + 6.564(7)	7)y + 6.164 (2)z =	= 11.604 (3)	
C5A—C1B	1.464 (2)	C5A' - C1B'	1.462 (2)	Deviation of stores for				
C1B - C2B	1.491 (2)	C1B' - C3B'	1.499 (2)	(* Denotes an atom inc	shuded in the calc	ulation of the lea	ist-squares ni	ane)
C1B - C3B	1.494 (2)	C1B - C2B C2B' - C2B'	1.501 (2)	(Denotes an atom inc	indea in the cale	diation of the lea	ist squares pr	anc)
C2D-C3D	1.473 (2)		1.473 (2)	Diimidazoquinazoline	group (rings C, L	D , <i>E</i> and <i>F</i>)		
C16 - N1 - C2	106.9(1)	C16' - N1' - C2'	107.0(1)	C6* 0	.044 (1)	C15*	-0.00	9 (1)
N1 - C2 - C3 N4 - C3 - C2	107.3(1)	N1 = C2 = C3 N4' = C3' = C2'	107.0(1) 101.1(1)	N7* 0	.046 (1)	C14*	0.02	0(1)
C5-N4-C16	122.8 (1)	C5' - N4' - C16'	123.1 (1)	C8* -0	.008 (1)	C13*	0.04	1 (1)
C5-N4-C3	127.4 (1)	C5'-N4'-C3'*	128.5(1)	N9* -0	.040(1)	C12*	0.014	4 (1) 8 (1)
C16-N4-C3	108.1(1)	C16'—N4'—C3'	108.3 (1)	C3* −0 N4* −0	0.010(1)	C10*	-0.03	B(1)
N4—C5—N9		N4' - C5' - N9'	117.4 (1)	C16* 0	.045(1)	010	0.05	<i>(</i> 1)
N4 - C5 - C6	117.5(1)				025(1)			
N4-C5-C0	117.5 (1) 136.5 (1)	N4'-C5'-C6'	136.7 (1)	C10 ⁻ 0	.025 (1)	61	0.00	4.72
N9-C5-C6	117.5 (1) 136.5 (1) 105.9 (1)	N4'	136.7 (1) 105.8 (1)	N1 0	.025 (1) .117 (2)	C2	0.084	4 (2)
N9-C5-C6 C5-C6-N7 C5-C6-C34	117.5 (1) 136.5 (1) 105.9 (1) 109.2 (1) 131.9 (1)	N4' - C5' - C6' N9' - C5' - C6' C5' - C6' - N7' C5' - C6' - N7'	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1)	N1 0 C3 0 Ovadiazole ring A	0.025 (1) 0.117 (2) 0.181 (2)	C2	0.084	4 (2)
N9-C5-C6 C5-C6-N7 C5-C6-C3A N7-C6-C3A	117.5 (1) 136.5 (1) 105.9 (1) 109.2 (1) 131.9 (1) 118.9 (1)	N4' -C5' -C6' N9' -C5' -C6' C5' -C6' -N7' C5' -C6' -C3A' N7' -C6' -C3A'	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1)	NI 0 C3 0 Oxadiazole ring A NIA 0	.025 (1) .117 (2) .181 (2) .295 (2)	C2 N4 <i>A</i>	0.08	4 (2) 2 (2)
N9-C5-C6 C5-C6-N7 C5-C6-C3A N7-C6-C3A C8-N7-C6	117.5 (1) 136.5 (1) 105.9 (1) 109.2 (1) 131.9 (1) 118.9 (1) 106.2 (1)	N4'-C5'-C6' N9'-C5'-C6' C5'-C6'-N7' C5'-C6'-C3A' N7'-C6'-C3A' C8'-N7'-C6'	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1)	N1 0 C3 0 Oxadiazole ring A 0 N1A 0 O2A 0	.025 (1) .117 (2) .181 (2) .295 (2) .259 (2)	C2 N4 <i>A</i> C5 <i>A</i>	0.084 0.022 0.14	4 (2) 2 (2) 8 (2)
N9-C5-C6 C5-C6-N7 C5-C6-C3A N7-C6-C3A C8-N7-C6 N7-C8-N9	117.5 (1) 136.5 (1) 105.9 (1) 109.2 (1) 131.9 (1) 118.9 (1) 106.2 (1) 112.3 (1)	$\begin{array}{c} N4' - C5' - C6' \\ N9' - C5' - C6' \\ C5' - C6' - N7' \\ C5' - C6' - C3A' \\ N7' - C6' - C3A' \\ C8' - N7' - C6' \\ N7' - C8' - N9' \end{array}$	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1)	N1 0 C3 0 Oxadiazole ring A 0 N1A 0 O2A 0 C3A 0	.025 (1) .117 (2) .181 (2) .295 (2) .259 (2) .093 (2)	C2 N4 <i>A</i> C5 <i>A</i>	0.084 0.022 0.144	4 (2) 2 (2) 8 (2)
N9-C5-C6 C5-C6-N7 C5-C6-C3A N7-C6-C3A C8-N7-C6 N7-C8-N9 C5-N9-C8	117.5 (1) 136.5 (1) 109.2 (1) 131.9 (1) 118.9 (1) 118.9 (1) 106.2 (1) 112.3 (1) 106.4 (1)	N4' - C5' - C6' N9' - C5' - C6' C5' - C6' - N7' C5' - C6' - C3A' N7' - C6' - C3A' C8' - N7' - C6' N7' - C8' - N9' C5' - N9' - C8'	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1) 106.4 (1)	NI 0 Oxadiazole ring A NIA 0 O2A 0 C3A 0 Cyclopropyl ring B	.025 (1) .117 (2) .181 (2) .295 (2) .259 (2) .093 (2)	C2 N4A C5A	0.084 0.022 0.144	4 (2) 2 (2) 8 (2)
$N_{2} = C_{5} = C_{6}$ $C_{5} = C_{6} = C_{7}$ $C_{5} = C_{6} = C_{3A}$ $N_{7} = C_{6} = C_{3A}$ $C_{8} = N_{7} = C_{6}$ $N_{7} = C_{8} = N_{9}$ $C_{5} = N_{9} = C_{10}$ $C_{8} = N_{9} = C_{10}$	117.5 (1) 136.5 (1) 109.2 (1) 131.9 (1) 118.9 (1) 106.2 (1) 112.3 (1) 106.4 (1) 124.1 (1)	$\begin{array}{c} N4' - C5' - C6' \\ N9' - C5' - C6' \\ C5' - C6' - N7' \\ C5' - C6' - C3a' \\ N7' - C6' - C3a' \\ C8' - N7' - C6' \\ N7' - C8' - N9' \\ C5' - N9' - C8' \\ C5' - N9' - C10' \\ C5' - N9' - C10' \\ C8' - N9' \\ C8' - N9' \\ C8' - N$	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1) 106.4 (1) 120.6 (1)	NI 0 Oxadiazole ring A NIA 0 O2A 0 C3A 0 Cyclopropyl ring B C1B 0	.025 (1) .117 (2) .181 (2) .295 (2) .259 (2) .093 (2) .144 (3)	C2 N4A C5A C3B	0.084 0.022 0.144 -0.786	4 (2) 2 (2) 8 (2) 6 (3)
N = -C5 - C6 $C5 - C6 - N7$ $C5 - C6 - C3A$ $N7 - C6 - C3A$ $C8 - N7 - C6$ $N7 - C6$ $N7 - C8 - N9$ $C5 - N9 - C10$ $C8 - N9 - C10$ $C11 - C15$	117.5 (1) 136.5 (1) 105.9 (1) 109.2 (1) 131.9 (1) 118.9 (1) 106.2 (1) 112.3 (1) 106.4 (1) 124.1 (1) 129.5 (1) 120.6 (1)	$\begin{array}{c} N4' - C5' - C6' \\ N9' - C5' - C6' \\ C5' - C6' - N7' \\ C5' - C6' - C3a' \\ N7' - C6' - C3a' \\ C8' - N7' - C6' \\ N7' - C8' - N9' \\ C5' - N9' - C8' \\ C5' - N9' - C10' \\ C5' - N9' - C10' \\ C8' - N9' - C10' \\ C11' - C10' - C15' \\ \end{array}$	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1) 106.4 (1) 124.1 (1) 129.5 (1) 120.8 (1)	N1 0 C3 0 Oxadiazole ring A 0 N1A 0 O2A 0 C3A 0 Cyclopropyl ring B 0 C1B 0 C2B 0	.025 (1) .117 (2) .181 (2) .295 (2) .259 (2) .093 (2) .144 (3) .656 (3)	C2 N4A C5A C3B	0.084 0.022 0.144 -0.786	4 (2) 2 (2) 8 (2) 6 (3)
N = -C5 - C6 $C5 - C6 - C3A$ $N7 - C6 - C3A$ $C8 - N7 - C6$ $C5 - N9 - C6$ $C5 - N9 - C8$ $C5 - N9 - C10$ $C8 - N9 - C10$ $C11 - C10 - C15$ $C11 - C10 - N9$	117.5 (1) 136.5 (1) 105.9 (1) 109.2 (1) 131.9 (1) 118.9 (1) 106.2 (1) 112.3 (1) 106.4 (1) 124.1 (1) 129.5 (1) 120.6 (1) 121.6 (1)	N4' - C5' - C6' N9' - C5' - C6' C5' - C6' - N7' C5' - C6' - C3A' N7' - C6' - C3A' C8' - N7' - C6' N7' - C8' - N9' C5' - N9' - C8' C5' - N9' - C10' C8' - N9' - C10' C11' - C10' - C15' C11' - C10' - N9'	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1) 124.1 (1) 129.5 (1) 120.8 (1) 121.2 (1)	N10C30Oxadiazole ring AN1A0O2A0C3A0Cyclopropyl ring BC1B0C2B0R.m.s. deviation of fitt	.025 (1) .117 (2) .181 (2) .259 (2) .259 (2) .093 (2) .144 (3) .656 (3) ed atoms from pl:	C2 N4A C5A C3B ane = 0.032 Å	0.084 0.022 0.144 -0.786	4 (2) 2 (2) 8 (2) 6 (3)
N = -C5 - C6 $C5 - C6 - C3A$ $N7 - C6 - C3A$ $N7 - C6 - C3A$ $C8 - N7 - C6$ $N7 - C8 - N9$ $C5 - N9 - C10$ $C8 - N9 - C10$ $C1 - C10 - C15$ $C11 - C10 - N9$ $C15 - C10 - N9$	117.5 (1) 136.5 (1) 105.9 (1) 109.2 (1) 131.9 (1) 118.9 (1) 106.2 (1) 112.3 (1) 106.4 (1) 124.1 (1) 129.5 (1) 120.6 (1) 121.6 (1) 117.9 (1)	$\begin{array}{c} N4' - C5' - C6' \\ N9' - C5' - C6' \\ C5' - C6' - N7' \\ C5' - C6' - C3A' \\ N7' - C6' - C3A' \\ C8' - N7' - C6' \\ N7' - C8' - N9' \\ C5' - N9' - C8' \\ C5' - N9' - C10' \\ C8' - N9' - C10' \\ C11' - C10' - C15' \\ C11' - C10' - N9' \\ C15' - C10' - N9' \end{array}$	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1) 106.4 (1) 124.1 (1) 129.5 (1) 120.8 (1) 121.2 (1) 118.2 (1)	C10* 0 N1 0 C3 0 Oxadiazole ring AN1A 0 O2A 0 C3A 0 Cyclopropyl ring BC1B 0 C2B 0 R.m.s. deviation of fittee	.025 (1) .117 (2) .181 (2) .295 (2) .259 (2) .093 (2) .144 (3) .656 (3) ed atoms from pl:	C2 N4A C5A C3B ane = 0.032 Å	0.084 0.022 0.144 -0.786	4 (2) 2 (2) 8 (2) 6 (3)
N = -C5 - C6 $C5 - C6 - C3A$ $N7 - C6 - C3A$ $N7 - C6 - C3A$ $C8 - N7 - C6$ $N7 - C8 - N9$ $C5 - N9 - C10$ $C8 - N9 - C10$ $C1 - C10 - C15$ $C11 - C10 - N9$ $C15 - C10 - N9$ $C15 - C10 - N9$ $C12 - C10 - N9$	117.5 (1) 136.5 (1) 105.9 (1) 109.2 (1) 131.9 (1) 118.9 (1) 106.2 (1) 112.3 (1) 106.4 (1) 124.1 (1) 129.5 (1) 120.6 (1) 121.6 (1) 117.9 (1) 119.4 (1)	$\begin{array}{c} N4' - C5' - C6' \\ N9' - C5' - C6' \\ C5' - C6' - N7' \\ C5' - C6' - C3A' \\ N7' - C6' - C3A' \\ C8' - N7' - C6' \\ N7' - C8' - N9' \\ C5' - N9' - C8' \\ C5' - N9' - C10' \\ C8' - N9' - C10' \\ C11' - C10' - C15' \\ C11' - C10' - N9' \\ C15' - C10' - N9' \\ C12' - C11' - C10' \\ \end{array}$	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1) 106.4 (1) 124.1 (1) 129.5 (1) 120.8 (1) 121.2 (1) 118.2 (1)	C10*0N10C30Oxadiazole ring AN1A0O2A0C3A0Cyclopropyl ring BC1B0C2B0R.m.s. deviation of fitteMolecule 1, oxadiaz	.025 (1) .117 (2) .181 (2) .259 (2) .259 (2) .093 (2) .144 (3) .656 (3) ed atoms from pl: cole ring A	C2 N4A C5A C3B ane = 0.032 Å	0.084 0.02 0.143 -0.786	4 (2) 2 (2) 8 (2) 6 (3)
N = -C5 - C6 $C5 - C6 - C3A$ $N7 - C6 - C3A$ $N7 - C6 - C3A$ $N7 - C6 - N9$ $C5 - N9 - C8$ $C5 - N9 - C10$ $C8 - N9 - C10$ $C1 - C10 - C15$ $C11 - C10 - N9$ $C15 - C10 - N9$ $C15 - C10 - N9$ $C12 - C10 - N9$ $C12 - C10 - C13$ $C11 - C10 - C13$ $C11 - C10 - C13$ $C11 - C10 - C13$ $C12 - C13 - C13$ $C11 - C10 - C13$	117.5 (1) 136.5 (1) 105.9 (1) 109.2 (1) 131.9 (1) 118.9 (1) 106.2 (1) 112.3 (1) 106.4 (1) 124.1 (1) 129.5 (1) 120.6 (1) 121.6 (1) 117.9 (1) 119.4 (1) 120.4 (1)	N4' - C5' - C6' N9' - C5' - C6' C5' - C6' - N7' C5' - C6' - C3A' N7' - C6' - C3A' N7' - C6' - C3A' C8' - N7' - C6' N7' - C8' - N9' - C10' C5' - N9' - C10' C1' - C10' - C15' C11' - C10' - N9' C15' - C10' - N9' C15' - C10' - N9' C12' - C11' - C10'	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1) 124.1 (1) 129.5 (1) 120.8 (1) 121.2 (1) 118.2 (1) 119.3 (1) 120.6 (2)	C10* 0 N1 0 C3 0 Oxadiazole ring AN1A 0 O2A 0 C3A 0 Cyclopropyl ring BC1B 0 C2B 0 R.m.s. deviation of fitteMolecule 1, oxadiazEmetion of class (1)	.025 (1) .117 (2) .181 (2) .295 (2) .259 (2) .093 (2) .144 (3) .656 (3) ed atoms from pla tole ring A	C2 N4A C5A C3B ane = 0.032 Å	0.08 0.02 0.14 -0.78	4 (2) 2 (2) 8 (2) 6 (3)
N = -C5 - C6 $C5 - C6 - C3A$ $N7 - C6 - C3A$ $N7 - C6 - C3A$ $N7 - C8 - N9$ $C5 - N9 - C8$ $C5 - N9 - C10$ $C1 - C10 - C15$ $C11 - C10 - N9$ $C15 - C10 - N9$ $C12 - C11 - C10$ $C11 - C10 - N9$ $C12 - C11 - C10$ $C11 - C10 - C13$ $C14 - C13 - C12$ $C13 - C14 - C15$	117.5 (1) 136.5 (1) 105.9 (1) 109.2 (1) 131.9 (1) 118.9 (1) 106.2 (1) 112.3 (1) 106.4 (1) 124.1 (1) 129.5 (1) 120.6 (1) 117.9 (1) 119.4 (1) 120.4 (1) 120.5 (1) 100.5 (1)	$\begin{array}{c} N4' - C5' - C6' \\ N9' - C5' - C6' \\ C5' - C6' - N7' \\ C5' - C6' - C3A' \\ N7' - C6' - C3A' \\ N7' - C6' - C3A' \\ C8' - N7' - C6' \\ N7' - C8' - N9' \\ C5' - N9' - C10' \\ C5' - N9' - C10' \\ C11' - C10' - C15' \\ C11' - C10' - N9' \\ C15' - C10' - N9' \\ C12' - C11' - C10' \\ C11' - C10' - N9' \\ C12' - C11' - C10' \\ C11' - C12' - C13' \\ C14' - C13' - C12' \\ C15' - C14' - C13' \\ C15' - C14' - C15' \\ C15' - C15' - C12' \\ C15' - C15' - C12' \\ C15' - C15' - C12' \\ C15' - C15' - C15' \\ C15' - C15' \\ C15' - C15' - C1$	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1) 124.1 (1) 129.5 (1) 120.8 (1) 121.2 (1) 119.3 (1) 120.6 (2) 120.3 (1)	C10* 0 N1 0 C3 0 Oxadiazole ring AN1A 0 O2A 0 C3A 0 Cyclopropyl ring BC1B 0 C2B 0 R.m.s. deviation of fitteMolecule 1, oxadiazEquation of plane: 6.4*	.025 (1) .117 (2) .181 (2) .295 (2) .259 (2) .093 (2) .144 (3) .656 (3) ed atoms from pla zole ring <i>A</i> 71 (4) <i>x</i> + 9.232 (1)	C2 N4 <i>A</i> C5 <i>A</i> C3 <i>B</i> ane = 0.032 Å	0.08 0.02 0.143 -0.786 = 12.633 (6)	4 (2) 2 (2) 8 (2) 6 (3)
N = -C5 - C6 $C5 - C6 - C34$ $N7 - C6 - C34$ $N7 - C6 - C34$ $N7 - C8 - N9$ $C5 - N9 - C8$ $C5 - N9 - C10$ $C1 - C10 - C15$ $C11 - C10 - N9$ $C15 - C10 - N9$ $C12 - C11 - C10$ $C11 - C12 - C13$ $C14 - C13 - C12$ $C13 - C14 - C15$ $C14 - C15 - C10$	117.5 (1) 136.5 (1) 105.9 (1) 109.2 (1) 131.9 (1) 118.9 (1) 106.2 (1) 112.3 (1) 106.4 (1) 124.1 (1) 129.5 (1) 120.6 (1) 117.9 (1) 119.4 (1) 120.4 (1) 120.5 (1) 119.8 (2) 119.2 (1)	$\begin{array}{c} N4' - C5' - C6' \\ N9' - C5' - C6' \\ C5' - C6' - N7' \\ C5' - C6' - C3A' \\ N7' - C6' - C3A' \\ N7' - C6' - C3A' \\ C8' - N7' - C6' \\ N7' - C8' - N9' - C10' \\ C5' - N9' - C10' \\ C5' - N9' - C10' \\ C11' - C10' - C15' \\ C11' - C10' - N9' \\ C15' - C10' - N9' \\ C12' - C11' - C10' \\ C11' - C12' - C13' \\ C14' - C13' - C12' \\ C13' - C14' - C15' \\ C14' - C15' - C10' \\ C10' - C10' - C15' \\ C14' - C15' - C10' \\ C10' - C10' - C10' \\ C11' - C10' - C15' \\ C10' - C10' - C15' \\ C10' - C15' - C10' \\ C10' - C10' - C10' \\ C10' - C15' - C10' \\ C10' - C15' - C10' \\ C10' - C10' - C10' \\ C10' - C15' - C10' \\ C10' - C10' \\ C10' - C10' - C10' \\ C10' - C10' - C10' \\ C10' - C10' \\ C10' - C$	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1) 124.1 (1) 129.5 (1) 120.8 (1) 121.2 (1) 119.3 (1) 120.6 (2) 120.3 (1) 119.8 (1) 119.8 (1)	C10*0N10C30Oxadiazole ring AN1A0O2A0C3A0Cyclopropyl ring BC1B0C2B0R.m.s. deviation of fittMolecule 1, oxadiazEquation of plane: 6.4*Deviation of atoms fro	.025 (1) .117 (2) .181 (2) .295 (2) .259 (2) .093 (2) .144 (3) .656 (3) ed atoms from pl: cole ring A 71 (4)x + 9.232 (1) m the plane (Å):	C2 N4 <i>A</i> C5 <i>A</i> C3 <i>B</i> ane = 0.032 Å 16)y + 6.656 (7)z	0.084 0.022 0.144 -0.786 = 12.633 (6)	4 (2) 2 (2) 8 (2) 6 (3)
$\begin{array}{c} N_{9} = -C_{5} = -C_{6} \\ C_{5} = -C_{6} = -C_{7} \\ C_{5} = -C_{6} = -C_{3} \\ N_{7} = -C_{6} = -C_{3} \\ C_{8} = -N_{7} = -C_{6} \\ N_{7} = -C_{8} = -N_{9} \\ C_{5} = -N_{9} = -C_{10} \\ C_{11} = -C_{11} \\ C_{11} = -C_{13} \\ C_{11} = -C_{13} \\ C_{11} = -C_{13} \\ C_{11} = -C_{15} \\ C_{11} = -C_{15} \\ C_{11} = -C_{10} \\ C_{11} = -C_{$	117.5 (1) 136.5 (1) 105.9 (1) 109.2 (1) 131.9 (1) 118.9 (1) 106.2 (1) 112.3 (1) 106.4 (1) 124.1 (1) 129.5 (1) 120.6 (1) 121.6 (1) 117.9 (1) 120.4 (1) 120.5 (1) 119.8 (2) 119.2 (1) 121.8 (1)	$\begin{array}{c} N4' - C5' - C6' \\ N9' - C5' - C6' \\ C5' - C6' - N7' \\ C5' - C6' - C3A' \\ N7' - C6' - C3A' \\ N7' - C8' - N9' \\ C5' - N9' - C10' \\ C5' - N9' - C10' \\ C5' - N9' - C10' \\ C11' - C10' - C15' \\ C11' - C10' - N9' \\ C12' - C11' - C10' \\ C11' - C10' - N9' \\ C12' - C11' - C10' \\ C11' - C12' - C13' \\ C11' - C13' - C12' \\ C13' - C14' - C15' \\ C14' - C15' - C10' \\ C14' $	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1) 124.1 (1) 129.5 (1) 120.8 (1) 121.2 (1) 119.3 (1) 120.6 (2) 120.3 (1) 119.8 (1) 119.1 (1) 121.7 (1)	N10C30Oxadiazole ring AN1A0O2A0C3A0Cyclopropyl ring BC1B0C2B0R.m.s. deviation of fitteMolecule 1, oxadiazEquation of plane: 6.4"Deviation of atoms fro(* Denotes an atom inc	.025 (1) .117 (2) .181 (2) .295 (2) .259 (2) .093 (2) .144 (3) .656 (3) ed atoms from pl: cole ring <i>A</i> 71 (4)x + 9.232 (1) m the plane (Å): .luded in the calc	C2 N4 A C5 A C3 B ane = 0.032 Å 16)y + 6.656 (7)z ulation of the lea	0.08 0.02 0.143 -0.786 = 12.633 (6)	4 (2) 2 (2) 8 (2) 6 (3)
$\begin{array}{c} N_{9} = -C_{5} = -C_{6} \\ C_{5} = -C_{6} = -C_{6} \\ C_{5} = -C_{6} = -C_{3} \\ N_{7} = -C_{6} = -C_{3} \\ C_{8} = -N_{7} = -C_{6} \\ N_{7} = -C_{8} = -N_{9} \\ C_{5} = -N_{9} = -C_{10} \\ C_{11} = -C_{10} = -C_{10} \\ C_{11} = -C_{11} = -C_{10} \\ C_{11} = -C_{11} = -C_{10} \\ C_{11} = -C_{15} = -C_{10} \\ C_{10} = -C_{15} = -C_{16} \\ C_{10} = -C_{15} \\ C_$	$\begin{array}{c} 117.5 (1) \\ 136.5 (1) \\ 105.9 (1) \\ 109.2 (1) \\ 131.9 (1) \\ 118.9 (1) \\ 106.2 (1) \\ 112.3 (1) \\ 106.4 (1) \\ 124.1 (1) \\ 129.5 (1) \\ 120.6 (1) \\ 121.6 (1) \\ 117.9 (1) \\ 120.5 (1) \\ 119.4 (1) \\ 120.5 (1) \\ 119.8 (2) \\ 119.2 (1) \\ 121.8 (1) \\ 119.0 (1) \end{array}$	$\begin{array}{c} N4' - C5' - C6' \\ N9' - C5' - C6' \\ C5' - C6' - N7' \\ C5' - C6' - C3A' \\ N7' - C6' - C3A' \\ N7' - C8' - N9' \\ C5' - N9' - C10' \\ C5' - N9' - C10' \\ C5' - N9' - C10' \\ C11' - C10' - C15' \\ C11' - C10' - N9' \\ C12' - C11' - C10' \\ C11' - C10' - N9' \\ C12' - C11' - C10' \\ C11' - C13' - C12' \\ C13' - C13' - C12' \\ C13' - C14' - C15' \\ C14' - C15' - C10' \\ C14' - C15' - C16' \\ C10' - C15' - C16' \\ \end{array}$	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1) 124.1 (1) 129.5 (1) 120.8 (1) 121.2 (1) 119.3 (1) 120.6 (2) 120.3 (1) 119.8 (1) 119.1 (1) 121.7 (1) 119.1 (1)	N10C30Oxadiazole ring ANIA0O2A0C3A0Cyclopropyl ring BC1B0C2B0R.m.s. deviation of fitteMolecule 1, oxadiazEquation of plane: 6.4"Deviation of atoms fro(* Denotes an atom income	.025 (1) .117 (2) .181 (2) .295 (2) .259 (2) .093 (2) .144 (3) .656 (3) ed atoms from plane cole ring <i>A</i> 71 (4)x + 9.232 (1) m the plane (Å): cluded in the calc	C2 N4 <i>A</i> C5 <i>A</i> C3 <i>B</i> ane = 0.032 Å 16)y + 6.656 (7)z ulation of the lea	0.08 0.02 0.143 -0.786 r = 12.633 (6) ust-squares pl	4 (2) 2 (2) 8 (2) 6 (3) ane)
$\begin{array}{c} N_{9} = -C_{5} = -C_{6} \\ C_{5} = -C_{6} = -C_{6} \\ C_{5} = -C_{6} = -C_{3} \\ N_{7} = -C_{6} = -C_{3} \\ C_{8} = -N_{7} = -C_{6} \\ N_{7} = -C_{8} = -N_{9} \\ C_{5} = -N_{9} = -C_{10} \\ C_{11} = -C_{10} = -C_{$	$\begin{array}{c} 117.5 (1)\\ 136.5 (1)\\ 105.9 (1)\\ 109.2 (1)\\ 131.9 (1)\\ 118.9 (1)\\ 106.2 (1)\\ 112.3 (1)\\ 106.4 (1)\\ 124.1 (1)\\ 129.5 (1)\\ 120.5 (1)\\ 121.6 (1)\\ 117.9 (1)\\ 120.5 (1)\\ 119.4 (1)\\ 120.5 (1)\\ 119.8 (2)\\ 119.2 (1)\\ 119.2 (1)\\ 119.5 (1)\\ \end{array}$	$\begin{array}{c} N4' - C5' - C6' \\ N9' - C5' - C6' \\ C5' - C6' - N7' \\ C5' - C6' - C3A' \\ N7' - C6' - C3A' \\ N7' - C6' - C3A' \\ C8' - N9' - C6' \\ N7' - C8' - N9' \\ C5' - N9' - C10' \\ C5' - N9' - C10' \\ C11' - C10' - C15' \\ C11' - C10' - N9' \\ C15' - C10' - N9' \\ C15' - C10' - N9' \\ C15' - C11' - C10' \\ C11' - C12' - C13' \\ C14' - C13' - C12' \\ C13' - C14' - C15' \\ C14' - C15' - C16' \\ C10' - C15' - C16' \\ N1' - C16' - N4' \\ \end{array}$	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1) 124.5 (1) 120.8 (1) 121.2 (1) 118.2 (1) 119.3 (1) 120.6 (2) 120.3 (1) 119.8 (1) 119.1 (1) 115.8 (1)	N10C30Oxadiazole ring AN1A0O2A0C3A0Cyclopropyl ring BC1B0C2B0R.m.s. deviation of fitteMolecule 1, oxadiazEquation of plane: 6.4"Deviation of atoms fro(* Denotes an atom incoOxadiazole ring A	.025 (1) .117 (2) .181 (2) .295 (2) .259 (2) .093 (2) .144 (3) .656 (3) ed atoms from plate cole ring <i>A</i> 71 (4)x + 9.232 (1) m the plane (Å): cluded in the calc	C2 N4 <i>A</i> C5 <i>A</i> C3 <i>B</i> ane = 0.032 Å (6)y + 6.656 (7)z ulation of the lea	0.08 0.02 0.143 -0.784 = 12.633 (6) ust-squares pl	4 (2) 2 (2) 8 (2) 6 (3) ane)
N=-C5C6 $C5C6C3A$ $N7C6C3A$ $R7C6C3A$ $C8N7C6$ $R7C8N9$ $C5N9C10$ $C11C10C15$ $C11C10C15$ $C11C10N9$ $C15C10N9$ $C12C11C10$ $C11C12C13$ $C14C15C16$ $C14C15C16$ $N1C16N4$ $N1C16N4$ $N1C16C15$	$\begin{array}{c} 117.5 (1) \\ 136.5 (1) \\ 105.9 (1) \\ 109.2 (1) \\ 131.9 (1) \\ 118.9 (1) \\ 106.2 (1) \\ 112.3 (1) \\ 106.4 (1) \\ 124.1 (1) \\ 129.5 (1) \\ 120.5 (1) \\ 120.5 (1) \\ 120.5 (1) \\ 119.4 (1) \\ 120.5 (1) \\ 119.8 (2) \\ 119.2 (1) \\ 119.2 (1) \\ 119.2 (1) \\ 119.5 (1) \\ 115.5 (1) \\ 126.2 (1) \\$	N4' - C5' - C6' N9' - C5' - C6' C5' - C6' - C3A' N7' - C6' - C3A' N7' - C6' - C3A' N7' - C8' - N9' C5' - N9' - C10' C5' - N9' - C10' C11' - C10' - N9' C15' - C10' - N9' C15' - C10' - N9' C15' - C10' - N9' C11' - C12' - C13' C14' - C13' - C12' C14' - C15' - C10' C14' - C15' - C10' C10' - C15' - C10'	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1) 124.5 (1) 129.5 (1) 120.8 (1) 121.2 (1) 118.2 (1) 119.3 (1) 120.6 (2) 120.3 (1) 119.8 (1) 119.1 (1) 119.1 (1) 115.8 (1) 126.1 (1)	N10C30Oxadiazole ring AN1A0O2A0C3A0Cyclopropyl ring BC1B0C2B0R.m.s. deviation of fitteMolecule 1, oxadiazEquation of plane: 6.4"Deviation of atoms fro(* Denotes an atom incoOxadiazole ring AN1A*0	$\begin{array}{c}$	C2 N4A C5A C3B ane = 0.032 Å I(6)y + 6.656 (7)z ulation of the lea N4A*	0.08 0.02 0.143 -0.784 r = 12.633 (6) ust-squares pl 0.000	4 (2) 2 (2) 8 (2) 6 (3) ane) 2 (1)
$\begin{array}{c} N_{9} = -C_{5} = -C_{6} \\ C_{5} = -C_{6} = -C_{3} \\ N_{7} = -C_{6} = -C_{3} \\ R_{8} = N_{7} = -C_{6} \\ N_{7} = -C_{8} = N_{9} \\ C_{5} = N_{9} = -C_{1} \\ R_{8} = N_{9} = -C_{1} \\ C_{1} = -C_{10} = -C_{15} \\ C_{11} = -C_{10} = -C_{13} \\ C_{12} = -C_{13} = -C_{12} \\ C_{13} = -C_{14} = -C_{15} \\ C_{14} = -C_{15} = -C_{16} \\ C_{10} = -C_{15} = -C_{16} \\ C_{10} = -C_{15} \\ N_{4} = -C_{16} \\ N_{4} = -C_{16}$	117.5 (1) 136.5 (1) 105.9 (1) 109.2 (1) 131.9 (1) 118.9 (1) 106.2 (1) 112.3 (1) 106.4 (1) 124.1 (1) 129.5 (1) 120.6 (1) 121.6 (1) 117.9 (1) 119.4 (1) 120.5 (1) 119.8 (2) 119.2 (1) 121.8 (1) 119.5 (1) 126.2 (1) 118.3 (1) 103.1 (1) 105.1 (1) 105.2 (1) 105.1 (1)	N4' - C5' - C6' N9' - C5' - C6' C5' - C6' - C3A' C5' - C6' - C3A' N7' - C6' - C3A' N7' - C6' - C3A' C5' - N9' - C6' N7' - C8' - N9' C5' - N9' - C10' C5' - N9' - C10' C11' - C10' - N9' C15' - C10' - N9' C15' - C10' - N9' C15' - C10' - N9' C12' - C11' - C10' C11' - C12' - C13' C14' - C13' - C10' C14' - C15' - C16' N1' - C16' - N4' N1' - C16' - C15' N4' - C16' - C15'	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1) 126.1 (1) 129.5 (1) 120.8 (1) 121.2 (1) 119.3 (1) 120.6 (2) 120.3 (1) 119.8 (1) 119.1 (1) 121.7 (1) 119.1 (1) 115.8 (1) 126.1 (1) 118.2 (1) 126.1 (1) 118.2 (1) 120.4 (1) 121.2 (1) 121.3 (1) 121.7 (1) 121.7 (1) 121.7 (1) 121.7 (1) 121.7 (1) 121.7 (1) 121.2 (1) 122.2 (1) 122	C10*0N10C30Oxadiazole ring AN1A0O2A0C3A0Cyclopropyl ring BC1B0C2B0R.m.s. deviation of fitteMolecule 1, oxadiazEquation of plane: 6.4*Deviation of atoms fro (* Denotes an atom incomeOxadiazole ring A N1A*N1A*0O24*0	$\begin{array}{c}$	C2 N4 <i>A</i> C5 <i>A</i> C3 <i>B</i> ane = 0.032 Å (6) <i>y</i> + 6.656 (7) <i>z</i> ulation of the lea N4 <i>A</i> * C5 <i>A</i> *	0.08 0.02 0.143 -0.786 = 12.633 (6) ust-squares pl 0.007 -0.007	4 (2) 2 (2) 8 (2) 6 (3) ane) 2 (1) 2 (1)
N=-C5C6 $C5C6C3A$ $N7C6C3A$ $C8N7C6$ $N7C8N9$ $C5N9C10$ $C8N9C10$ $C11C10C15$ $C11C10C15$ $C11C10N9$ $C15C10N9$ $C15C10N9$ $C12C11C10$ $C14C15C10$ $C14C15C16$ $C10C15C16$ $C10C15C16$ $C10C15C16$ $C10C15C16$ $N1C16N4$ $N1C16C15$ $C5AN1AO2A$ $C34O2AN1A$	$\begin{array}{c} 117.5 (1) \\ 136.5 (1) \\ 105.9 (1) \\ 109.2 (1) \\ 131.9 (1) \\ 118.9 (1) \\ 118.9 (1) \\ 106.2 (1) \\ 112.3 (1) \\ 106.4 (1) \\ 124.1 (1) \\ 129.5 (1) \\ 120.5 (1) \\ 121.6 (1) \\ 117.9 (1) \\ 119.4 (1) \\ 120.4 (1) \\ 120.5 (1) \\ 119.2 (1) \\$	N4' - C5' - C6' N9' - C5' - C6' C5' - C6' - C3A' C5' - C6' - C3A' N7' - C6' - C3A' N7' - C6' - C3A' C8' - N9' - C6' N7' - C8' - N9' C5' - N9' - C10' C11' - C10' - C15' C11' - C10' - N9' C15' - C10' - N9' C15' - C10' - N9' C15' - C10' - N9' C12' - C11' - C10' C11' - C12' - C13' C14' - C13' - C10' C14' - C15' - C10' C14' - C15' - C10' C14' - C15' - C16' N1' - C16' - N4' N1' - C16' - C15' N4' - C16' - C15' C34' - O24' - N14'	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1) 126.1 (1) 129.5 (1) 120.8 (1) 121.2 (1) 119.3 (1) 120.6 (2) 120.3 (1) 119.8 (1) 119.1 (1) 121.7 (1) 119.5 (1) 121.7 (1) 119.5 (1) 126.1 (1) 118.2 (1) 103.0 (1) 103.0 (1) 106.1 (1)	N1 0 C3 0 Oxadiazole ring A N1A 0 O2A 0 C3A 0 Cyclopropyl ring B C1B 0 C2B 0 R.m.s. deviation of fitte Molecule 1, oxadiaz Equation of plane: 6.4 ² Deviation of atoms fro (* Denotes an atom inc Oxadiazole ring A N1A* 0 O2A* 0 Cyclopropyl ring B Caller of the second sec	.025 (1) $.117 (2)$ $.181 (2)$ $.295 (2)$ $.259 (2)$ $.093 (2)$ $.144 (3)$ $.656 (3)$ ed atoms from plane (Å): cole ring A 71 (4)x + 9.232 (1) m the plane (Å): cluded in the calc .001 (1) $.000 (1)$	C2 N4 <i>A</i> C5 <i>A</i> C3 <i>B</i> ane = 0.032 Å 16)y + 6.656 (7) <i>z</i> ulation of the lea N4 <i>A</i> * C5 <i>A</i> *	0.084 0.022 0.144 -0.786 = 12.633 (6) ust-squares pl 0.002 -0.002	4 (2) 2 (2) 8 (2) 6 (3) () ane) 2 (1) 2 (1)
N=-C5-C6 $C5-C6-N7$ $C5-C6-C3A$ $N7-C6-C3A$ $C8-N7-C6$ $N7-C8-N9$ $C5-N9-C10$ $C8-N9-C10$ $C11-C10-C15$ $C11-C10-N9$ $C15-C10-N9$ $C15-C10-N9$ $C15-C10-N9$ $C12-C11-C10$ $C14-C15-C10$ $C14-C15-C16$ $C14-C15-C16$ $C10-C15-C16$ $C14-C15-C16$ $C10-C15-C16$ $C14-C15-C16$ $C10-C15-C16$ $C14-C15-C16$ $C10-C15-C16$ $C14-C15-C16$ $C10-C15-C16$ $C14-C15-C16$ $C14-C15-C16$ $C14-C15-C16$ $C10-C15-C16$ $C14-C15-C16$ $C14-C15-C1$	117.5 (1) 136.5 (1) 105.9 (1) 109.2 (1) 131.9 (1) 118.9 (1) 106.2 (1) 112.3 (1) 106.4 (1) 124.1 (1) 129.5 (1) 120.6 (1) 121.6 (1) 119.4 (1) 120.4 (1) 120.5 (1) 119.2 (1) 121.8 (1) 119.0 (1) 115.5 (1) 126.2 (1) 118.3 (1) 103.1 (1) 106.3 (1) 112.8 (1)	$\begin{array}{c} N4' - C5' - C6' \\ N9' - C5' - C6' \\ C5' - C6' - N7' \\ C5' - C6' - C3A' \\ N7' - C6' - C3A' \\ N7' - C6' - C3A' \\ C8' - N7' - C6' \\ N7' - C8' - N9' - C10' \\ C5' - N9' - C10' \\ C5' - N9' - C10' \\ C11' - C10' - C15' \\ C11' - C10' - N9' \\ C15' - C10' - N9' \\ C15' - C10' - N9' \\ C12' - C11' - C10' \\ C11' - C12' - C13' \\ C14' - C13' - C12' \\ C13' - C14' - C15' \\ C14' - C15' - C16' \\ C10' - C15' - C16' \\ N1' - C16' - C15' \\ N1' - C16' - C15' \\ N4' - C16' - C15' \\ C3A' - N1A' - O2A' \\ C3A' - O2A' - N1A' \\ N4A' - C3A' - O2A' \\ \end{array}$	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1) 129.5 (1) 120.8 (1) 121.2 (1) 119.3 (1) 120.6 (2) 120.3 (1) 119.8 (1) 119.1 (1) 119.1 (1) 112.6 (1) 118.2 (1) 119.2 (1) 113.2 (1) 113.2 (1) 113.8 (1) 123.0 (1) 103.0 (1) 106.1 (1) 112.8 (1)	C10*0N10C30Oxadiazole ring AN1A0O2A0C3A0Cyclopropyl ring BC1B0C2B0R.m.s. deviation of fitteMolecule 1, oxadiazoleEquation of plane: 6.4*Deviation of atoms fro(* Denotes an atom incoOxadiazole ring AN1A*0O2A*0C3A*-0Cyclopropyl ring BC1B0	$\begin{array}{c}$	C2 N4A C5A C3B ane = 0.032 Å 16)y + 6.656 (7)z ulation of the lea N4A* C5A* C3B	0.084 0.022 0.144 -0.786 = 12.633 (6) ust-squares pl 0.002 -0.002 -0.784	4 (2) 2 (2) 8 (2) 6 (3) () ane) 2 (1) 2 (1) 5 (3)
$\begin{array}{c} N_{9} = -C_{5} = -C_{6} \\ C_{5} = -C_{6} = -C_{3A} \\ N_{7} = -C_{6} = -C_{3A} \\ C_{8} = -N_{7} = -C_{6} \\ N_{7} = -C_{8} = -N_{9} \\ C_{5} = -N_{9} = -C_{10} \\ C_{10} = -C_{10} \\ C_{11} = -C_{10} = -C_{15} \\ C_{11} = -C_{10} = -N_{9} \\ C_{11} = -C_{10} = -N_{10} \\ C_{11} = -C_{10} = -C_{15} \\ C_{14} = -C_{15} = -C_{16} \\ C_{10} = -C_{15} = -C_{16} \\ C_{10} = -C_{15} \\ C_{5A} = -O_{2A} = -N_{1A} \\ N_{4A} = -C_{3A} = -O_{2A} \\ N_{4A} = -C_{3A} = -C_{6} \\ \end{array}$	$\begin{array}{c} 117.5 (1)\\ 136.5 (1)\\ 105.9 (1)\\ 109.2 (1)\\ 131.9 (1)\\ 118.9 (1)\\ 118.9 (1)\\ 106.2 (1)\\ 112.3 (1)\\ 106.4 (1)\\ 124.1 (1)\\ 129.5 (1)\\ 120.6 (1)\\ 121.6 (1)\\ 121.6 (1)\\ 121.6 (1)\\ 119.4 (1)\\ 120.4 (1)\\ 120.4 (1)\\ 120.5 (1)\\ 119.8 (2)\\ 119.2 (1)\\ 121.8 (1)\\ 119.0 (1)\\ 115.5 (1)\\ 126.2 (1)\\ 118.3 (1)\\ 103.1 (1)\\ 106.3 (1)\\ 112.8 (1)\\ 131.2 (1)\\ \end{array}$	$\begin{array}{c} N4' - C5' - C6' \\ N9' - C5' - C6' \\ C5' - C6' - N7' \\ C5' - C6' - C3A' \\ N7' - C6' - C3A' \\ N7' - C6' - C3A' \\ C8' - N7' - C6' \\ N7' - C8' - N9' - C10' \\ C5' - N9' - C10' \\ C5' - N9' - C10' \\ C11' - C10' - C15' \\ C11' - C10' - N9' \\ C15' - C10' - N9' \\ C12' - C11' - C10' \\ C11' - C12' - C13' \\ C14' - C13' - C12' \\ C14' - C15' - C10' \\ C14' - C15' - C10' \\ C14' - C15' - C16' \\ C10' - C15' - C16' \\ C16' - C15' - C15' \\ C14' - C15' - C15' \\ C14' - C15' - C16' \\ C10' - C15' - C15' \\ N1' - C16' - C15' \\ C5A' - N1A' - O2A' \\ N4A' - C3A' - O2A' \\ N4A' - C3A' - O2A' \\ \end{array}$	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1) 106.4 (1) 129.5 (1) 120.8 (1) 121.2 (1) 119.3 (1) 120.6 (2) 120.3 (1) 119.8 (1) 119.1 (1) 119.1 (1) 115.8 (1) 126.1 (1) 118.2 (1) 103.0 (1) 106.1 (1) 113.8 (1) 120.8 (1) 122.8 (1) 130.5 (1)	C10*0N10C30Oxadiazole ring AN1A0O2A0C3A0Cyclopropyl ring BC1B0C2B0R.m.s. deviation of fitthMolecule 1, oxadiazEquation of plane: 6.4*Deviation of atoms fro(* Denotes an atom incoOxadiazole ring AN1A*0O2A*0C3A*-0Cyclopropyl ring BC1B0C2B0	.025 (1) $.117 (2)$ $.181 (2)$ $.295 (2)$ $.259 (2)$ $.093 (2)$ $.144 (3)$ $.656 (3)$ ed atoms from platic from platic from platic from platic from platic from platic from the plane $(Å)$: cluded in the calc $.001 (1)$ $.000 (1)$ $.001 (1)$ $.017 (3)$ $.682 (3)$	C2 N4A C5A C3B ane = 0.032 Å (6)y + 6.656 (7)z ulation of the lea N4A* C5A* C3B	0.08 0.02 0.141 -0.786 = 12.633 (6) ust-squares pl 0.000 -0.000 -0.000	4 (2) 2 (2) 8 (2) 6 (3) () ane) 2 (1) 2 (1) 5 (3)
N=-C5C6 $C5C6C3A$ $N7C6C3A$ $C8N7C6C3A$ $C8N7C6$ $N7C8N9$ $C5N9C10$ $C8N9C10$ $C11C10C15$ $C11C10C15$ $C11C10N9$ $C15C10N9$ $C15C10N9$ $C12C11C10$ $C14C15C16$ $C14C15C16$ $C14C15C16$ $C14C15C16$ $C14C15C16$ $C10C15C16$ $N1C16N4$ $N1C16N4$ $N1C16C15$ $N4C16C15$ $N4C16C15$ $C5AN1AO2A$ $N4AC3AO2A$ $N4AC3AO2A$ $N4AC3AC6$ $O2AC3AC6$ $O2AC3AC6$	$117.5 (1) \\ 136.5 (1) \\ 105.9 (1) \\ 109.2 (1) \\ 131.9 (1) \\ 118.9 (1) \\ 118.9 (1) \\ 106.2 (1) \\ 112.3 (1) \\ 106.4 (1) \\ 124.1 (1) \\ 129.5 (1) \\ 120.6 (1) \\ 121.6 (1) \\ 121.6 (1) \\ 117.9 (1) \\ 119.4 (1) \\ 120.4 (1) \\ 120.4 (1) \\ 120.5 (1) \\ 119.2 (1) \\ 119.2 (1) \\ 119.2 (1) \\ 115.5 (1) \\ 126.2 (1) \\ 118.3 (1) \\ 103.1 (1) \\ 106.3 (1) \\ 112.8 (1) \\ 131.2 (1) \\ 115.9 (1) \\ 115.9 (1) \\ 100.1 \\ 115.9 (1) \\ 100.1 \\ 115.9 (1) \\ 100.1 \\ 115.9 (1) \\ 100.1 \\ 115.9 (1) \\ 100.1 \\ 110.1 \\ 100.1 \\ 110.$	$\begin{array}{c} N4' - C5' - C6' \\ N9' - C5' - C6' \\ C5' - C6' - N7' \\ C5' - C6' - C3A' \\ N7' - C6' - C3A' \\ N7' - C6' - C3A' \\ C8' - N7' - C6' \\ N7' - C8' - N9' - C10' \\ C5' - N9' - C10' \\ C1' - C10' - C15' \\ C11' - C10' - N9' \\ C15' - C10' - N9' \\ C12' - C11' - C10' \\ C11' - C10' - N9' \\ C12' - C11' - C10' \\ C11' - C10' - N9' \\ C12' - C11' - C10' \\ C11' - C12' - C13' \\ C14' - C13' - C12' \\ C13' - C14' - C15' \\ C14' - C15' - C16' \\ C10' - C15' - C16' \\ C16' - C15' - C15' \\ C5A' - N1A' - O2A' \\ N4A' - C3A' - O2A' \\ N4A' - C3A' - C6' * \\ O2A' - C3A' - C6' * \\ \end{array}$	136.7 (1) 105.8 (1) 109.4 (1) 131.7 (1) 119.0 (1) 106.0 (1) 112.4 (1) 106.4 (1) 129.5 (1) 120.8 (1) 121.2 (1) 119.3 (1) 120.6 (2) 120.3 (1) 119.8 (1) 119.1 (1) 121.7 (1) 119.1 (1) 115.8 (1) 126.1 (1) 118.2 (1) 103.0 (1) 105.5 (1) 116.7 (1)	C10*0N10C30N1A0O2A0C3A0Cyclopropyl ring BC1B0C2B0R.m.s. deviation of fitteMolecule 1, oxadiazEquation of plane: 6.4*Deviation of atoms fro(* Denotes an atom incoOxadiazole ring AN1A*0O2A*0C3A*-0Cyclopropyl ring BC1B0C2B0	$\begin{array}{c}$	C2 N4A C5A C3B ane = 0.032 Å 16)y + 6.656 (7)z ulation of the lea N4A* C5A* C3B	0.08 0.02 0.141 -0.786 = 12.633 (6) ust-squares pl 0.000 -0.0002 -0.782	4 (2) 2 (2) 8 (2) 6 (3) () ane) 2 (1) 2 (1) 5 (3)

Molecule 1, cyclopropyl ring B

Equation of plane: 5.477 (10)x - 3.285 (36)y + 10.022 (12)z = 6.077 (24)

Interplanar dihedral angles in molecule 1 (°)

Diimidazoquinazoline ring-oxadiazole ring	7.08 (7)
Diimidazoquinazoline ring-cyclopropyl ring	82.64 (7)
Oxadiazole ring-cyclopropyl ring	85.82 (7)

Molecule 2, diimidazoquinazoline group

Equation of plane: 6.833(1)x + 0.446(7)y + 7.203(2)z = 6.311(2)

Deviation of atoms from the plane (Å):

(* Denotes an atom included in the calculation of the least-squares plane) Distribution of the least-squares plane C_{1}^{\prime} D_{1}^{\prime} D_{2}^{\prime} D_{3}^{\prime} D_{4}^{\prime}

Dumidazoqu	iinazoline group (rings C	$\mathcal{L}, \mathcal{D}, \mathcal{E}$ and \mathcal{F}	
C6'*	-0.043 (1)	C15'*	0.033 (1)
N7'*	0.001 (1)	C14'*	0.029(1)
C8'*	0.051 (1)	C13'*	-0.015(1)
N9'*	0.036(1)	C12'*	-0.056(1)
C5'*	-0.021(1)	C11'*	-0.018(1)
N4'*	-0.044 (1)	C10'*	0.026(1)
C16'*	0.021 (1)		
N1′	0.036 (2)	C2′	-0.045 (2)
C3′	-0.036 (2)		
Oxadiazole 1	ring A'		
N1A'	-0.242 (2)	N4A'	-0.263(2)
02A'	-0.101 (2)	C5A'	-0.332(2)
C3A'	-0.130 (2)		
Cyclopropyl	ring B'		
C1 <i>B</i> ′	-0.506 (3)	C3B'	-1.386(3)
C2B'	0.076 (3)		

R.m.s. deviation of fitted atoms from plane = 0.034 Å

Molecule 2, oxadiazole ring A'

Equation of plane: 7.175 (3)x + 2.605 (18)y + 6.404 (7)z = 7.031 (6)

Deviation of atoms from the plane (Å):

(* Denotes an atom included in the calculation of the least-squares plane)

Oxadiazole ri	ng A'		
N1A'*	0.000(1)	N4A'*	0.002(1)
02A'*	0.002(1)	C5A'*	-0.001 (1)
C3A'*	-0.002(1)		
Cyclopropyl i	ring B'		
C1B	-0.017 (3)	C3B	-0.816(4)
C2B	0.658 (4)		

R.m.s. deviation of fitted atoms from plane = 0.002 Å

Molecule 2, cyclopropyl ring B'

Equation of plane: 4.745 (11)x - 4.318 (36)y + 10.659 (10)z = 9.760 (13)

Interplanar dihedral angles in molecule 2 (°)

Diimidazoquinazoline ring-oxadiazole ring	6.24 (7)
Diimidazoquinazoline ring-cyclopropyl ring	85.63 (6)
Oxadiazole ring-cyclopropyl ring	89.49 (7)

Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL92* (Sheldrick, 1992). Molecular graphics: *SNOOP1* (Davies, 1982).

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: LI1112). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Polymorph (II) of Methyl 3-(4-Ethoxy- α -hydroxyiminobenzyl)-1,2,2-trimethylcyclopentanecarboxylate

J. NURIT,* J. RAMBAUD, B. PAUVERT AND A. TÉROL

Laboratoire de Chimie Physique Générale, 15, Avenue Charles Flahaut, Faculté de Pharmacie, 34060 Montpellier CEDEX 1, France

P. CHEVALLET AND O. DOUMBIA

Laboratoire de Chimie Thérapeutique, Université Montpellier I, France

J.-P. DECLERCQ

Laboratoire de Chimie Physique et de Cristallographie, Université Catholique de Louvain, Belgium

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Abstract

The title compound, $C_{19}H_{27}NO_4$, is an intermediate product in the synthesis of oxazepinic and piperidinic compounds. Two crystalline forms of the title compound have been obtained but only one [form (II)] gave suitable crystals for X-ray structure analysis. The five-membered ring has an envelope conformation with C(2) 0.60 (5) Å out of the plane defined by the other four atoms. It has been established that the oxime group has a *syn* conformation and the two enantiomers form a dimer around the centre of symmetry by means of hydrogen bonds between their oxime groups.

Comment

The starting material for the synthesis of these oximes is camphoric anhydride (Chevallet *et al.*, 1988). Recrystallization of methyl 3-(4-ethoxy- α -hydroxyiminobenzyl)-1,2,2-trimethylcyclopentane-