observed [C2—Te1—C11—C12 = −94·3 (5), C2—Te1—C11—C16 = 86·7 (5), C2—Te3—C31—C32 = 34·3 (6) and C2—Te3—C31—C36 = −150·6 (5)°]. Also bond lengths found for Te3 are shorter than for Te1. Taking into account the ligand distribution and following the ideas of Husebye (1983), we presume that the Te1 lone non-bonding pairs occupy octahedral positions above and below the coordination plane whereas the Te3 lone pairs occupy equatorial positions together with C2 in a trigonal bipyramidal arrangement.

Financial support from the European Economic Community (MdM, Research Fellowship) is gratefully acknowledged. MdM is especially grateful to Instituto de Ciencia de Materiales de Barcelona (CSIC) where this work was developed.

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Acta Cryst. (1991). C**47**, 1266–1269

Structures of *N*-Substituted 1,2-Oxazines. II. Bicyclic Bridged Derivatives

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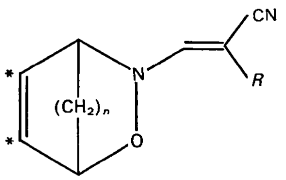
(*Received* 1 *May* 1990; *accepted* 18 *October* 1990)

Abstract. (I) 2-(2-Oxa-3-azabicyclo[2.2.2]oct-5-en-3-yl)-1,1-ethylenedicarbonitrile, $C_{10}H_9N_3O$, M_r = 187·20, orthorhombic, *Pnam*, a = 8·933 (1), b = 13·088 (1), c = 8·002 (2) Å, V = 935·6 (3) Å^3, Z = 4, D_x = 1·33 g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, μ = 7·5 cm^{-1}, F(000) = 392, T = 291 K, R = 0·056 for 642 observed reflections. (II) 2-(*tert*-Butylthio)-3-(2-oxa-3-azabicyclo[2.2.2]octan-3-yl)acrylonitrile, $C_{13}H_{20}N_2OS$, M_r = 252·38, monoclinic, $P2_1$, a = 12·098 (4), b = 17·770 (5), c = 10·926 (5) Å, β = 112·44 (3)°, V = 2171 (1) Å^3, Z = 6, D_x = 1·16 g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, μ = 2·1 cm^{-1}, F(000) = 816, T = 291 K, R = 0·064 for 3441 observed reflections. (III) 2-(*tert*-Butylthio)-3-(6-oxa-7-azabicyclo[3.2.2]non-8-en-7-yl)acrylonitrile, $C_{14}H_{20}N_2OS$, M_r = 264·39, orthorhombic, $P2_12_12_1$, a = 9·962 (3), b = 12·576 (3), c = 11·766 (4) Å, V = 1474·1 (7) Å^3, Z = 4, D_x = 1·19 g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, μ = 2·10 cm^{-1}, F(000) = 568, T = 291 K, R = 0·051 for 1259 observed reflections. The *E* configuration of the double bond is observed for both (II) and (III). Some geometrical parameters indicate clearly that the conjugation between the olefin and the ring system is less in molecule (III) than in the other two derivatives.

Introduction. A series of *N*-substituted bicyclic 1,2-oxazines has been synthetized and their thermal isomerization in epoxy-epimines has been studied (Vaerman, 1989).



n = 0 to 3; R = CN or S^{t}Bu; * single bond in (II)

With the aim of quantifying the effects of the bridge length (n) and that of the substituent (R) of the olefin on the geometry, we have determined the

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X-ray structures of some of these 1,2-oxazines. In this second paper, we report on the structures of three bridged bicyclo compounds: (I) 2-(2-oxa-3-azabicyclo[2.2.2]oct-5-en-3-yl)-1,1-ethylenedicarbonitrile ($n = 2$, $R = \mathrm{CN}$), (II) 2-(*tert*-butylthio)-3-(2-oxa-3-azabicyclo[2.2.2]octan-3-yl)acrylonitrile ($n = 2$, $R = \mathrm{S}^t\mathrm{Bu}$), (III) 2-(*tert*-butyltio)-3-(6-oxa-7-azabicyclo[3.2.2]non-8-en-7-yl)acryonitrile ($n = 3$, $R = \mathrm{S}^t\mathrm{Bu}$).

Experimental. The different data-collection and refinement parameters are summarized in Table 1. Compound (I) was recrystallized from acetone, (II) and (III) from diethyl ether. Lattice parameters refined using 15 reflections in the range $5 \leq 2\theta \leq 30°$. Huber diffractometer for (I), Syntex $P2_1$ diffractometer for (II) and (III), graphite-monochromatized Cu $K\alpha$ for (I), Mo $K\alpha$ for (II) and (III). One standard reflection checked every 50 reflections: no significant deviation. All three structures solved by *SHELXS*86 (Sheldrick, 1985). Three H atoms in (I), eight in (II), from difference Fourier syntheses, all the other H atoms calculated (C—H = 1·08 Å, H—C—H = 109·5°). Anisotropic least-squares refinement (*SHELX*76; Sheldrick, 1976) using *F*; H atom isotropic with common refined temperature factor. The structure of (I) was first solved in space group $Pna2_1$ with the whole molecule in the asymmetric part of the unit cell. The *N*-substituent was coplanar with C1, O2, N3 and C4 and it bisected the bicyclo system. So space group *Pnam* with a disordered bridge (as a simultaneous single and a double bond between C5 and C6) could be choosen after a shift of the origin by 0·25*z*. The disordered H's of CH=CH and $\mathrm{CH_2}$—$\mathrm{CH_2}$ were included with fixed positions and an occupation factor of 0·5. In structure (II), there are three independent molecules of which the third one (*C*) has some atoms with high *B* values (see Table 2). The maximum residual density peak was found in this agitated region and also the maximum shift to error was on U_{23} of atom C17*C*. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV).

Discussion. The final atomic coordinates for the non-H atoms are given in Table 2* for (I), (II) and (III) respectively. Figs. 1(*a*), 1(*b*) and 1(*c*) are stereoscopic drawings of the molecules showing the numbering of the atoms (*PLUTO*; Motherwell & Clegg, 1978).

The first point of interest was to establish the configuration of the double bond for (II) and (III).

Table 1. *Data collection and refinement parameters*

	(I)	(II)	(III)
Crystal size (mm)	0·22 × 0·11 × 0·07	0·32 × 0·42 × 0·65	0·32 × 0·27 × 0·20
$(\sin\sigma/\lambda)_{\max}$ (Å^{-1})	0·60	0·62	0·65
Range of *hkl*	$0 \leq h \leq 10$	$0 \leq h \leq 14$	$0 \leq h \leq 12$
	$0 \leq k \leq 15$	$0 \leq k \leq 21$	$0 \leq k \leq 16$
	$0 \leq l \leq 9$	$-13 \leq l \leq 12$	$0 \leq l \leq 15$
Indices of standard reflection	031	150	060
Number of measured reflections	910	4415	1939
Number of observed reflections $[I > 2{\cdot}5\sigma(I)]$	642	3441	1259
Number of parameters	85	461	191
R	0·056	0·064	0·051
wR	0·063	0·066	0·061
g $[w = 1/(\sigma^2 + gF^2)]$	0·00097	0·00010	0·00418
S	2·28	3·13	1·03
(Δ/σ)	0·03	0·86	0·19
$\Delta\rho_{\max,\min}$ (e Å^{-3})	0·25, −0·21	0·62, −0·27	0·28, −0·22

As shown on Figs. 1(*b*) and 1(*c*), it was *E* for both compounds. Thus in the three derivatives a cyano group is located on the same side as the O atom of the oxazine. This cyano group is essentially coplanar with the N—O bond in all the three molecules. In (I), the atoms N, O, C=C and CN are coplanar because of symmetry; they deviate from their best mean plane by less than 0·07 Å in (II)* and (III). The angles N—C=C and C=C—CN are significantly enlarged (average values of 129·7 and 125·9°, respectively, see Table 3) because of the steric repulsion. The same situation, with the same enlargement of the angles, was also observed in the *Z* monocyclic derivative 2-(*tert*-butylthio)-3-(3,6-dihydro-2*H*-1,2-oxazin-2-yl)acrylonitrile where S and O atoms interact (Tinant & Declercq, 1991).

Another point of interest is the degree of conjugation between the olefin and the N—O bond from one molecule to the other. The hybridization of the *N*-oxazine atom can be estimated by the sum of the angles around it and by its deviation from the plane passing through its three neighbour atoms. The angles around N are listed in Table 3; the sum of these angles is 360·0 for (I), 354·5 for (II) and 348·3° for (III). The deviations of N from the plane through C*c*, O and C*v*† are 0 for (I), 0·18 for (II) and 0·28 Å for (III). These values indicate a more pyramidal N atom for (III).

A lesser conjugation in molecule (III) is also clearly apparent from some of the bond length values (Table 3). The N—C*v* and C—CN single bonds are about 0·05 Å shorter, and the C=C bond 0·04 Å longer in (I) and (II) than in (III). The electrons are thus far more delocalized along ON—C=C—CN in (I) and (II) but also in the monocyclic derivative

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53673 (40 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

* As the three independent molecules of (II) have similar geometries, only mean values of the parameters will be considered in the following discussion.

† C*c* and C*v* denote C of the cyclic and vinyl systems, respectively.

Table 2. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic temperature factors* (Å^2)

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

	x	*y*	*z*	U_{eq}
Compound (I)				
C1	2224 (5)	7910 (3)	2500	0·050 (1)
O2	1237 (3)	8817 (2)	2500	0·065 (1)
N3	2125 (4)	9696 (2)	2500	0·052 (1)
C4	3754 (4)	9487 (3)	2500	0·044 (1)
C5	4073 (4)	8860 (3)	4051 (5)	0·060 (1)
C6	3188 (4)	7949 (2)	4042 (4)	0·058 (1)
C9	1462 (5)	10573 (3)	2500	0·046 (1)
C10	−45 (5)	10797 (3)	2500	0·051 (1)
C11	−452 (3)	11854 (2)	2500	0·053 (1)
N12	−773 (5)	12696 (3)	2500	0·070 (1)
C13	−1243 (5)	10092 (3)	2500	0·061 (1)
N14	−2264 (5)	9575 (3)	2500	0·095 (2)
Compound (II)				
C1*A*	2250 (6)	5530 (4)	4171 (7)	0·064 (1)
O2*A*	3149 (4)	5986 (3)	3956 (4)	0·081 (1)
N3*A*	2879 (5)	6018 (4)	2574 (5)	0·077 (2)
C4*A*	1797 (5)	5639 (5)	1764 (6)	0·067 (2)
C5*A*	1910 (8)	4805 (5)	2130 (9)	0·088 (2)
C6*A*	2207 (9)	4759 (5)	3581 (8)	0·094 (2)
C7*A*	1047 (7)	5892 (5)	3505 (9)	0·090 (2)
C8*A*	765 (7)	5978 (5)	2056 (9)	0·093 (2)
C9*A*	3732 (5)	6257 (4)	2205 (6)	0·050 (1)
C10*A*	4817 (5)	6559 (3)	2943 (6)	0·047 (1)
C11*A*	5262 (6)	6700 (4)	4328 (7)	0·056 (1)
N12*A*	5693 (5)	6839 (5)	5454 (7)	0·086 (2)
S13*A*	5762 (1)	6825	2139 (2)	0·053 (1)
C14*A*	6733 (5)	6005 (4)	2281 (6)	0·054 (1)
C15*A*	5998 (7)	5326 (4)	1691 (10)	0·085 (2)
C16*A*	7456 (7)	6224 (5)	1461 (9)	0·085 (1)
C17*A*	7562 (8)	5880 (7)	3691 (8)	0·110 (3)
C1*B*	6178 (7)	3335 (4)	3089 (8)	0·071 (2)
O2*B*	6640 (4)	3434 (2)	2071 (5)	0·065 (1)
N3*B*	6550 (4)	2748 (3)	1380 (5)	0·056 (1)
C4*B*	5778 (5)	2209 (4)	1659 (6)	0·053 (1)
C5*B*	4609 (6)	2609 (5)	1453 (7)	0·071 (2)
C6*B*	4857 (7)	3241 (5)	2433 (9)	0·084 (2)
C7*B*	6780 (7)	2657 (5)	3930 (7)	0·078 (2)
C8*B*	6371 (6)	1943 (4)	3073 (6)	0·064 (2)
C9*B*	7515 (5)	2542 (4)	1143 (5)	0·046 (1)
C10*B*	8511 (5)	2953 (4)	1291 (6)	0·051 (1)
C11*B*	8765 (5)	3695 (4)	1828 (7)	0·061 (2)
N12*B*	9041 (6)	4293 (4)	2238 (8)	0·093 (2)
S13*B*	9518 (2)	2566 (1)	656 (2)	0·070 (1)
C14*B*	10723 (6)	2163 (4)	2036 (8)	0·071 (2)
C15*B*	11451 (8)	2747 (6)	3010 (10)	0·113 (3)
C16*B*	10248 (10)	1620 (7)	2795 (11)	0·139 (4)
C17*B*	11521 (7)	1767 (7)	1464 (10)	0·130 (3)
C1*C*	4125 (8)	61 (5)	2286 (11)	0·100 (3)
O2*C*	5294 (5)	−61 (3)	2372 (6)	0·080 (1)
N3*C*	5651 (6)	−796 (3)	2789 (8)	0·086 (2)
C4*C*	4696 (8)	−1230 (5)	3023 (12)	0·099 (3)
C5*C*	4338 (8)	−845 (8)	3967 (8)	0·109 (3)
C6*C*	4039 (12)	−96 (7)	3571 (14)	0·151 (5)
C7*C*	3341 (11)	−483 (10)	1326 (10)	0·186 (5)
C8*C*	3683 (11)	−1276 (7)	1744 (11)	0·129 (4)
C9*C*	6464 (7)	−1083 (4)	2413 (10)	0·091 (2)
C10*C*	7149 (6)	−756 (4)	1803 (8)	0·067 (2)
C11*C*	7092 (6)	13 (4)	1405 (7)	0·062 (2)
N12*C*	7112 (5)	599 (4)	1022 (6)	0·074 (2)
S13*C*	8197 (2)	−1320 (1)	1446 (2)	0·085 (1)
C14*C*	9609 (7)	−1208 (5)	2859 (8)	0·075 (2)
C15*C*	9874 (13)	−478 (8)	3283 (17)	0·305 (7)
C16*C*	10519 (9)	−1688 (8)	2671 (10)	0·141 (4)
C17*C*	9444 (11)	−1525 (11)	4055 (12)	0·185 (6)
Compound (III)				
C1	−2675 (6)	4580 (5)	2898 (6)	0·060 (1)
C2	−4044 (6)	4117 (6)	2700 (6)	0·075 (2)
C3	−4551 (7)	3337 (7)	3622 (8)	0·079 (2)
C4	−3610 (7)	2424 (5)	3890 (6)	0·068 (2)
C5	−2153 (7)	2756 (5)	3976 (5)	0·057 (1)
O6	−1631 (4)	2850 (3)	2799 (4)	0·062 (1)
N7	−1644 (5)	3886 (4)	2357 (4)	0·054 (1)
C8	−2269 (7)	4649 (5)	4128 (6)	0·065 (2)
C9	−1957 (8)	3754 (6)	4622 (6)	0·071 (2)
C10	−406 (5)	4265 (4)	2082 (4)	0·046 (1)
C11	777 (5)	3779 (4)	2095 (4)	0·045 (1)
C12	1035 (7)	2762 (5)	2615 (5)	0·057 (1)
N13	1330 (7)	1972 (5)	3001 (6)	0·085 (2)
S14	2209 (2)	4442 (1)	1574 (1)	0·055 (1)
C15	2511 (5)	3834 (4)	172 (4)	0·050 (1)
C16	1324 (10)	4008 (9)	−591 (7)	0·115 (3)
C17	2785 (13)	2669 (6)	284 (7)	0·116 (3)
C18	3755 (9)	4390 (7)	−277 (7)	0·100 (3)

(Tinant & Declercq, 1991), than in (III). Nevertheless the N—O bond seems unaffected as its length is similar in all the compounds, ranging from 1·397 to 1·411 Å. This is very short for a N—O bond as we have shown (Tinant & Declercq, 1991).

It may be asked whether the conjugation is so different in molecule (III) compared with the others. Considering (II) and (III) for which the substitution and the configuration of the olefin are identical, only the different bridge length can be considered. Indeed molecule (II) is obviously more rigid than (III) and this is reflected in the torsion angles about N—O, 25° in (III) as compared to about 5° in (II). However as we have mentioned above the atoms involved in the conjugated pathway are coplanar in both molecules. A non-negligible twist of the double bond is nevertheless only observed in (III) where the torsion angle N—C═C—CN is −12° (compensated by O—N—C═C at 5° otherwise the atoms would not be coplanar).

Only the conformation of the [3.2.2] bicyclic system in (III) is worth a comment. The endocyclic torsion angles are: for C1—C2—C3—C4—C5—N6—O7, 91, −54, 43, −80, 97, −25 and −61°; for C1—C2—C3—C4—C5—C9═C8, −27, −54, 43, 44, −75, −6 and 73°; for C1—N7—O6—C5—C9═

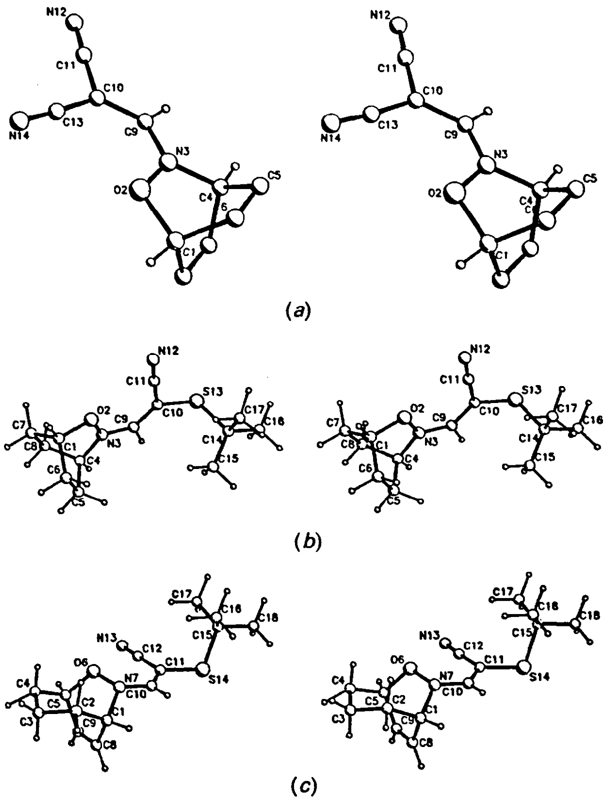

Fig. 1. Stereoscopic views of (*a*) compound (I), (*b*) compound (II) and (*c*) compound (III).

C8, 63, −25, −28, 46, −6 and −47°. Because of the bridge, the six-membered ring is inevitably a boat conformation but it is highly distorted in the C5—O6—N7 region. Concerning the two seven-membered rings, that with a C8—C9 double bond has a nearly regular boat conformation (Hendrickson's theoretical values: −30·9, −57·5, 57·5, 30·9, −69·9, 0, 69·9°) while that containing N—O is a distorted chair, particularly around N—O (theoretical values: 83·5, −63·8, 63·8, −83·5, 66·1, 0, −66·1°) (Hendrickson, 1967).

Table 3. *Selected bond distances* (Å) *and bond angles* (°)

	(I)	(II)*	(III)
N—O	1·397 (4)	1·411 (7)	1·403 (6)
N—*Cc*†	1·481 (5)	1·459 (10)	1·490 (7)
N—*Cv*†	1·292 (5)	1·319 (10)	1·362 (7)
Cv═*Cv*	1·378 (6)	1·368 (10)	1·328 (8)
C—CN	1·430 (6) 1·413 (6)	1·425 (10)	1·440 (9)
C≡N	1·139 (5) 1·136 (6)	1·148 (10)	1·131 (8)
Cv—S	—	1·760 (8)	1·763 (5)
O—N—*Cc*	113·9 (3)	113·2 (6)	113·1 (4)
O—N—*Cv*	118·2 (3)	116·4 (6)	113·9 (4)
Cc—N—*Cv*	127·9 (3)	124·9 (6)	121·3 (5)
Cc—O—N	108·9 (3)	109·3 (5)	114·6 (4)
N—*Cv*—*Cv*	129·5 (4)	129·7 (6)	129·8 (5)
Cv—*Cv*—CN	117·0 (4) 126·9 (4)	125·8 (7)	124·9 (5)
Cv—*Cv*—S	—	118·2 (5)	119·8 (4)

* Mean values over the three independent molecules.
† *Cc* for C of the ring, *Cv* for C of the vinyl part.

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Acta Cryst. (1991). C**47**, 1269–1271

Structure of 4,5,6,7-Tetrahydro-1,3-benzimidazole-2-thione

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(*Received* 9 *May* 1990; *accepted* 22 *October* 1990)

Abstract. $C_7H_{10}N_2S$, $M_r = 154{\cdot}23$, tetragonal, $P4_32_12$, $a = 7{\cdot}1519(6)$, $c = 14{\cdot}3532(6)$ Å, $V = 734{\cdot}2$ Å^3, $Z = 4$, $D_m = 1{\cdot}40$, $D_x = 1{\cdot}395$ Mg m^{-3}, $\lambda(\mathrm{Cu}\,K\alpha) = 1{\cdot}5418$ Å, $\mu = 3{\cdot}19$ mm^{-1}, $F(000) = 328$, $T = 296$ K, final $R = 0{\cdot}026$ for 520 observed reflections. The molecule has a crystallographic two-fold axis of symmetry. Both the S and the C atom bonded to it lie on this twofold axis, which also bisects the C(2)—C(2′) and C(4)—C(4′) bonds. The exocyclic C—S forms the thione structure in the solid state. The five-membered imidazole ring is planar, with the S atom also lying in this plane, whereas the cyclohexene ring has a distorted half-chair conformation. There is a relatively weak but linear hydrogen bond from the N—H group to the S atom of an adjacent molecule along **c**. Each S atom, because of its location on a twofold axis, is involved in two such bonds.

Introduction. The imidazolethione system has been a subject of interest on account of its wide-ranging pharmacological activity (Kohn, Kohn, Steenberg & Buckley, 1977; Gosselin, Imbach, Townsend & Panzica, 1979) and its effective inhibition of metallic corrosion (Donnelly, Downie, Grzeskowiak, Hamburg & Short, 1978). 4,5,6,7-Tetrahydro-1,3-benzimidazole-2-thione is one such compound newly synthesized by the reaction between potassium thiocyanate and 2-aminocyclohexanone oxime; the latter's amino N atom, acting as an electrophile, and its C atom bonded to the hydroxyimino group, acting

0108-2701/91/061269-03$03.00