during the desulfuration of (I) and an 18-membered heterocyclic macro-ring is created. It seems that it is not possible to close the central ring of (II) by an —O1—C1— bridge [the C4···C6 and C3···C7 distances in (III) are 4·637 (3) and 3·640 (3) Å respectively].

The molecule lies on a special position: a crystallographic twofold axis passes through the centre of the heterocyclic ring. The 18-membered heterocyclic ring has a 'saddle'-like conformation forced by two diimino fragments and four fused benzene rings. The molecule as a whole has the same conformation, but even more pronounced with the benzene rings lengthening the form of a 'saddle' (see Fig. 1). The diimide systems have noteworthy geometry. This is a significant distortion from linearity: the valence angle at C5 is 168·0 (2)° and the C=N distance is 1·214 (2) Å.

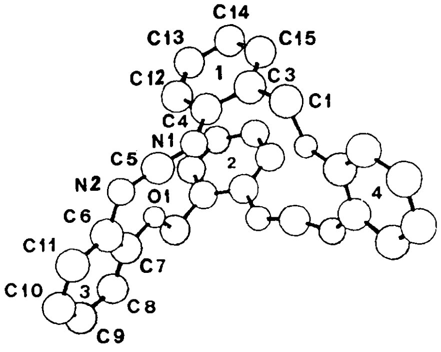

Fig. 1. The molecular structure showing the atom- and ring-numbering scheme.

It is remarkable that benzene rings 1 and 2 are nearly parallel to each other; the least-squares planes form an angle of 0·21 (7)°. The dihedral angle between benzene-ring planes 3 and 4 is 78·13 (5)°, and those between planes 1 and 3 and 1 and 4 are 108·24 (6) and 108·10 (6)°, respectively.

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Structure of *N*-(2-Phenylethenyl)pyrrolidin-2-one

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Abstract. $C_{12}H_{13}NO$, $M_r = 187{\cdot}2$, orthorhombic, *Pbca*, $a = 10{\cdot}896\ (3)$, $b = 8{\cdot}033\ (2)$, $c = 23{\cdot}376\ (8)$ Å, $V = 2046\ (1)$ Å^3, $Z = 8$, $D_x = 1{\cdot}216$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ Å, $\mu = 0{\cdot}072$ mm^{-1}, $F(000) = 800$, room temperature, final $R = 0{\cdot}058$ for 1290 observed reflections. The ethylene group of the title compound has a *trans* configuration and is antiperiplanar to the amide system of the lactam ring. The five-membered lactam ring is nearly planar with a mean deviation of 0·005 Å from the plane. The crystal structure is stabilized by weak intermolecular H···O interactions between the vinylic β-H atom and the carbonyl O atom of the next molecule, with a distance of 2·59 Å.

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Introduction. PE spectroscopy is a valuable method for conformational analysis of several compounds with suitable electronic structures (Klessinger & Rademacher, 1979). For enamines various investigations based on PE spectroscopy (Brown, 1976; Domelsmith, Houk & Rouge, 1977; Müller, Previdoli & Desilvestro, 1981; Lafon, Gonbeau, Pfister-Guillouzo, Lasne, Ripoll & Denis, 1986), semi-empirical calculations (Müller & Brown, 1978; Saebö & Radom, 1982) and structural studies (Brown, Damm, Dunitz, Eschenmoser, Hobi & Kratky, 1978) show for most investigated compounds that the N atom is sp^3 hybridized. While optimal n_N/π_{CC} conjugation in enamines is not possible, conformational analyses of the amide linkage (Kitano & Kuchitsu, 1974; Hoesterey, Neely & Worley, 1983; Norskov-Lauritsen, Bürgi, Hofmann & Schmidt, 1985; Treschanke & Rademacher, 1985; Marstokk, Möllendal, Samdal & Uggerud, 1989) have revealed an sp^2-hybridized N atom, which favours the conjugation.

The combination of an enamine with a cyclic amide (lactam) leads to an *N*-(1-alkenyl)lactam. Investigations of unsubstituted (Woydt, Rademacher, Kaupp & Sauerland, 1989) and substituted *N*-alkenyllactams by PE spectroscopy and semi-empirical calculations (*AM*1; Stewart, 1989) have shown that the two functional groups are coplanar. MNDO results support a pyramidal arrangement of the nitrogen substituents in the most stable form. To determine the structure, especially of monosubstituted *N*-(1-alkenyl)lactams, an X-ray analysis of the title compound has been performed. For the electronic structure of *N*-(2-phenylethenyl)pyrrolidin-2-one the torsional angles of the ethenyl and phenyl groups are of prominent interest.

Experimental. *N*-(2-Phenylethenyl)pyrrolidin-2-one was synthesized (Zezza & Smith, 1987) by condensation of 8·50 g (0·100 mol) pyrrolidin-2-one and 11·7 ml (0·100 mol) phenylacetaldehyde in the presence of 0·05 g *p*-toluenesulfonic acid. The reaction mixture was heated in toluene in a Dean–Stark apparatus for about 16 h. The solvent was evaporated and crystals were purified by recrystallization from ethyl acetate. Crystal size 0·35 × 0·6 × 0·8 mm, Nicolet *R*3*m* four-circle diffractometer, ω scan (scan width 1·20°, scan rate 1·50–14·65° $\min^{-1}$, depending on intensity), lattice parameters determined with angle positions of 50 reflections ($20{\cdot}0 \leq 2\theta \leq 25{\cdot}0°$). No absorption correction applied, max. value of $(\sin\theta)/\lambda = 0{\cdot}59$ Å^{-1}, 3864 measured reflections, *hkl* range $0 \leq h \leq 12$, $-9 \leq k \leq 9$ and $-27 \leq l \leq 0$, three check reflections with no significant intensity variation, 1791 independent intensities ($R_{\rm int} = 0{\cdot}039$), 1290 observed reflections [$F_o \geq 3{\cdot}0\sigma(F_o)$]. Structure solved by direct methods and full-matrix refinement on F_o with *SHELXTL-Plus* (Sheldrick, 1988). All non-H atoms had anisotropic displacement parameters. H atoms, found in $\Delta\rho$ map, were refined in calculated positions using a rigid model with fixed isotropic temperature factors (C—H 0·96 Å, H—C—H 109·5° for methylene), 127 parameters refined, $R = 0{\cdot}058$ and $wR = 0{\cdot}066$ with $w^{-1} = [\sigma^2(F_o) + 0{\cdot}0005F_o^2]$, $(\Delta/\sigma)_{\max} = 0{\cdot}001$, max. and min. electron densities based on final difference Fourier synthesis $(\Delta\rho)_{\max} = 0{\cdot}15$ and $(\Delta\rho)_{\min} = -0{\cdot}22$ e Å^{-3}, atomic scattering factors from *SHELXTL-Plus* (Sheldrick, 1988).

Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic displacement factors* (Å$^2 \times 10^3$)

	x	y	z	$U_{\rm eq}$
N(1)	8817 (2)	2016 (2)	4599 (1)	58 (1)
C(2)	8020 (2)	1757 (3)	4161 (1)	61 (1)
O(2)	7034 (2)	1052 (3)	4208 (1)	89 (1)
C(3)	8553 (3)	2465 (4)	3626 (1)	73 (1)
C(4)	9782 (2)	3196 (4)	3792 (1)	70 (1)
C(5)	9921 (3)	2902 (3)	4436 (1)	67 (1)
C(11)	8563 (2)	1496 (3)	5155 (1)	61 (1)
C(12)	9277 (2)	1776 (3)	5606 (1)	60 (1)
C(13)	9013 (2)	1189 (3)	6193 (1)	57 (1)
C(14)	7998 (2)	246 (3)	6340 (1)	68 (1)
C(15)	7816 (3)	−303 (3)	6896 (1)	73 (1)
C(16)	8654 (3)	108 (3)	7315 (1)	79 (1)
C(17)	9660 (3)	1051 (4)	7182 (1)	79 (1)
C(18)	9843 (3)	1598 (3)	6626 (1)	69 (1)

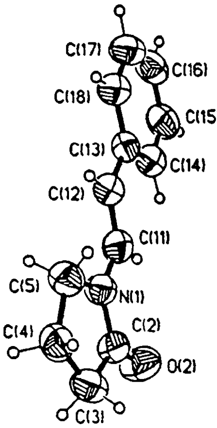

Fig. 1. Perspective view of the molecule showing the atomic labelling. Ellipsoids are drawn to include 50% probability for non-H atoms.

Discussion. Final atomic coordinates and equivalent isotropic thermal parameters are listed in Table 1.* Selected bond lengths and angles are given in Table 2. The numbering scheme and the geometry of the molecule are shown in Fig. 1.

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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 54330 (10 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond lengths* (Å), *bond angles* (°) *and selected torsional angles* (°)

N(1)—C(2)	1·359 (3)	C(12)—C(13)	1·479 (3)
N(1)—C(5)	1·448 (3)	C(13)—C(14)	1·383 (4)
N(1)—C(11)	1·392 (3)	C(13)—C(18)	1·397 (4)
C(2)—O(2)	1·219 (3)	C(14)—C(15)	1·386 (4)
C(2)—C(3)	1·492 (4)	C(15)—C(16)	1·380 (4)
C(3)—C(4)	1·513 (4)	C(16)—C(17)	1·368 (4)
C(4)—C(5)	1·530 (4)	C(17)—C(18)	1·385 (4)
C(11)—C(12)	1·330 (3)		
C(2)—N(1)—C(5)	114·0 (2)	C(11)—C(12)—C(13)	124·6 (2)
C(2)—N(1)—C(11)	122·0 (2)	C(12)—C(13)—C(14)	124·1 (2)
C(5)—N(1)—C(11)	124·0 (2)	C(12)—C(13)—C(18)	118·1 (2)
N(1)—C(2)—O(2)	124·5 (2)	C(14)—C(13)—C(18)	117·8 (2)
N(1)—C(2)—C(3)	108·9 (2)	C(13)—C(14)—C(15)	121·4 (2)
O(2)—C(2)—C(3)	126·6 (2)	C(14)—C(15)—C(16)	119·7 (3)
C(2)—C(3)—C(4)	106·1 (2)	C(15)—C(16)—C(17)	120·0 (3)
C(3)—C(4)—C(5)	106·3 (2)	C(16)—C(17)—C(18)	120·3 (3)
N(1)—C(5)—C(4)	104·7 (2)	C(13)—C(18)—C(17)	120·8 (3)
N(1)—C(11)—C(12)	124·9 (2)		
C(5)—N(1)—C(2)—O(2)	−179·3 (2)	N(1)—C(11)—C(12)—C(13)	−178·6 (2)
C(5)—N(1)—C(2)—C(3)	0·9 (3)	C(11)—C(12)—C(13)—C(14)	1·4 (4)
C(11)—N(1)—C(2)—O(2)	−0·6 (4)	C(11)—C(12)—C(13)—C(18)	−179·2 (2)
C(11)—N(1)—C(2)—C(3)	179·6 (2)	C(12)—C(13)—C(14)—C(15)	178·4 (2)
N(1)—C(2)—C(3)—C(4)	−0·1 (3)	C(18)—C(13)—C(14)—C(15)	−1·1 (4)
O(2)—C(2)—C(3)—C(4)	−179·9 (3)	C(13)—C(14)—C(15)—C(16)	0·7 (4)
C(2)—C(3)—C(4)—C(5)	−0·7 (3)	C(14)—C(15)—C(16)—C(17)	−0·1 (4)
C(2)—N(1)—C(5)—C(4)	−1·3 (3)	C(15)—C(16)—C(17)—C(18)	0·0 (4)
C(11)—N(1)—C(5)—C(4)	−180·0 (2)	C(12)—C(13)—C(18)—C(17)	−178·5 (3)
C(3)—C(4)—C(5)—N(1)	1·2 (3)	C(14)—C(13)—C(18)—C(17)	1·0 (4)
C(2)—N(1)—C(11)—C(12)	−176·9 (2)	C(16)—C(17)—C(18)—C(13)	−0·5 (4)
C(5)—N(1)—C(11)—C(12)	1·7 (4)		

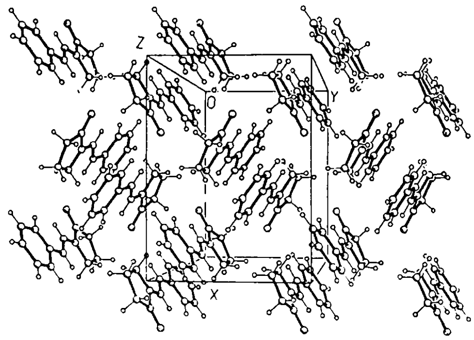

Fig. 2. Perspective view showing the crystal packing along the *x* axis. The broken lines represent H···O interactions.

The ethenylene group of the title compound is antiperiplanar to the amide linkage with a torsional angle of −176·9 (2)°. Also the phenyl group is coplanar with the enamide linkage. The five-membered lactam ring is planar with a mean deviation of 0·005 Å. The N atom has a planar surrounding (sum of angles 360·0°). This structure shows an optimal conjugation of the π-electron system.

The length of the carbonyl bond [1·219 (3) Å] of the title compound corresponds exactly to the standard value for this kind of bond (Rademacher, 1987). In *N*-(3-methyl-1-butenyl)piperidin-2-one (Woydt, Rademacher, Brett & Boese, 1991) the C=O bond is 0·03 Å longer than the standard length. The vinylic C(11)—C(12) bond length of 1·330 (3) Å is only 0·01 Å shorter than the standard length. The vinyl group in *N*-(3-methyl-1-butenyl)piperidin-2-one is 0·02 Å and in *N*-ethenylphthalimide (Kaupp & Matthies, 1988) 0·047 Å shorter than the standard C=C length. These results show, that the enamide–phenyl conjugation compensates for the inductive effect of the carbonyl O atom.

The observed structure is in accord with the PE spectrum of the title compound, which shows a large splitting of the π-electron ionization potentials. In Fig. 2 the crystal packing of the title compound is shown. Between the vinylic β-H atom and the carbonyl O atom of the next molecule a distance of 2·59 Å indicates a weak intermolecular H···O interaction.

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