O(17) and N(1). This interaction does not result in any severe changes in torsion angles.

The heterocyclic *D* ring is *cis*-fused to ring *C* and 1,3-diaxially fused to ring *E*. Alternatively, it can be considered to be a component of a bridged eight-membered ring. There are several opposing interactions which determine the torsion angles in the heterocyclic six-membered ring. The fusion of the C(4a) and C(3) axial substituents tends to increase the torsion angles while interactions $H(4\alpha)\cdots H(15\gamma) = 2{\cdot}04$, $H(11a)\cdots H(15\gamma) = 2{\cdot}33$ and $H(12\beta)\cdots N(1) = 2{\cdot}72$ Å tend to flatten the ring and reduce the torsion angles.

Ring *E* is *cis*-fused to ring *C* and 1,3-diaxially fused to ring *D*. The diaxial fusion and interactions $H(12\alpha)\cdots H(16\gamma) = 2{\cdot}51$, $H(12\beta)\cdots N(1) = 2{\cdot}72$ and $H(13)\cdots H(14\beta) = 2{\cdot}23$ Å determine the variations in torsion angles. The eight-membered ring assumes a boat conformation. The H on O(17) is bonded intramolecularly to N(1) with $N(1)\cdots O(17) = 2{\cdot}763$, $N(1)\cdots H(17) = 2{\cdot}11$ and $H(17)\cdots O(17) = 0{\cdot}87$ Å. O(18) is intermolecularly hydrogen bonded to N(6) with $N(6)\cdots O(18) = 2{\cdot}891$, $N(6)\cdots H(18) = 2{\cdot}18$ and $H(18)\cdots O(18) = 0{\cdot}87$ Å.

Aristotelinine can be considered a biological oxidation product of aristoteline. These alkaloids represent a unique structural type which may be restricted to the genus *Aristotelia*.

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2,3-Dihydro-2-(4-methoxyphenyl)-3-phenyl-4*H*-1,3,2-benzoxazaphosphorine-4-thione 2-Oxide

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Abstract. $C_{20}H_{16}NO_3PS$, $M_r = 381{\cdot}4$, monoclinic, $P2_1/c$, $a = 12{\cdot}96$ (2), $b = 15{\cdot}60$ (2), $c = 9{\cdot}49$ (1) Å, $\beta = 103{\cdot}8$ (2)°, $V = 1863{\cdot}3$ Å^3, $Z = 4$, $D_c = 1{\cdot}36$ g cm^{-3}. Refinement gave $R = 0{\cdot}056$ and $R_w = 0{\cdot}060$ for 235 parameters and 1761 significant reflexions $[I > 3\sigma(I)]$. The stereochemistry of the molecule has been established.

Introduction. The title compound was prepared by Scheibye, Pedersen & Lawesson (1978*a*,*b*) as yellow crystals (m.p. 173 °C). The crystals were kindly provided by S. Scheibye.

A crystal 1·0 × 0·7 × 0·2 mm was mounted about **c**. The lattice type and space group were established from photographs taken with Cu and Mo radiations.

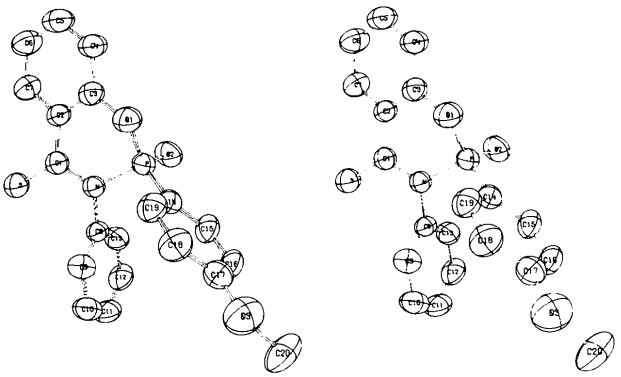

Fig. 1. A stereoscopic drawing of the molecule showing the numbering of the atoms.

Table 1. *Fractional atomic coordinates* (×10^4) *and their e.s.d.'s*

	x	*y*	*z*
S	5117 (2)	437 (1)	2642 (2)
P	8131 (1)	840 (1)	5527 (2)
O(1)	7659 (4)	1649 (3)	6195 (5)
O(2)	8902 (4)	1033 (3)	4687 (5)
O(3)	9426 (4)	−1490 (3)	10506 (5)
N	6987 (4)	409 (3)	4490 (5)
C(1)	6116 (5)	882 (4)	3803 (7)
C(2)	6155 (6)	1806 (4)	4152 (7)
C(3)	6898 (6)	2161 (4)	5299 (7)
C(4)	6918 (6)	3019 (5)	5657 (8)
C(5)	6160 (7)	3553 (5)	4810 (10)
C(6)	5421 (7)	3222 (5)	3655 (10)
C(7)	5414 (6)	2368 (5)	3337 (8)
C(8)	7085 (5)	−496 (4)	4157 (6)
C(9)	6643 (6)	−1106 (5)	4859 (7)
C(10)	6782 (7)	−1971 (5)	4591 (8)
C(11)	7351 (7)	−2200 (5)	3617 (9)
C(12)	7784 (6)	−1590 (6)	2911 (9)
C(13)	7662 (6)	−731 (5)	3183 (7)
C(14)	8544 (5)	155 (4)	7030 (6)
C(15)	9428 (5)	−361 (5)	7150 (7)
C(16)	9745 (5)	−921 (4)	8280 (7)
C(17)	9183 (5)	−961 (4)	9347 (7)
C(18)	8293 (6)	−442 (5)	9240 (7)
C(19)	7977 (5)	111 (5)	8103 (8)
C(20)	10250 (7)	−2131 (5)	10575 (9)

Intensities were collected on a computer-controlled Supper diffractometer with graphite-monochromated Mo $K\alpha$ radiation, a scintillation counter and a pulse-height analyser. 4366 independent reflexions were measured by the background–peak–background method out to $\sin\theta = 0{\cdot}5$. 1761 significant reflexions with $I > 3\sigma(I)$ were used in the subsequent calculations. No correction was applied for absorption.

The structure was determined with *MULTAN* (Germain, Main & Woolfson, 1971). Coordinates, anisotropic thermal parameters and a scale factor were refined by full-matrix least-squares calculations. The positions of 13 H atoms attached to the aromatic rings were calculated and included in the refinement but the geometrical and thermal parameters of the H atoms were not refined. The final $R = 0{\cdot}056$ and $R_w = 0{\cdot}060$ for 235 parameters and 1761 significant reflexions $[I > 3\sigma(I)]$. Atomic coordinates are listed in Table 1.*

Table 2. *Bond lengths* (Å) *and their e.s.d.'s*

P–N	1·710 (6)	C(8)–C(9)	1·363 (9)
N–C(1)	1·376 (8)	C(9)–C(10)	1·394 (10)
C(1)–C(2)	1·477 (9)	C(10)–C(11)	1·361 (11)
C(2)–C(3)	1·385 (9)	C(11)–C(12)	1·360 (12)
C(3)–O(1)	1·391 (8)	C(12)–C(13)	1·382 (10)
O(1)–P	1·599 (5)	C(13)–C(8)	1·369 (9)
P–O(2)	1·451 (5)	C(14)–C(15)	1·383 (9)
P–C(14)	1·760 (7)	C(15)–C(16)	1·368 (9)
N–C(8)	1·459 (8)	C(16)–C(17)	1·383 (10)
C(1)–S	1·641 (7)	C(17)–C(18)	1·393 (9)
C(3)–C(4)	1·380 (10)	C(18)–C(19)	1·365 (10)
C(4)–C(5)	1·388 (11)	C(19)–C(14)	1·393 (9)
C(5)–C(6)	1·373 (11)	C(17)–O(3)	1·351 (8)
C(6)–C(7)	1·365 (11)	O(3)–C(20)	1·453 (9)
C(7)–C(2)	1·391 (10)		

Table 3. *Angles* (°) *and their e.s.d.'s*

O(1)–P–N	100·2 (3)	C(5)–C(6)–C(7)	120·7 (8)
O(1)–P–O(2)	115·6 (3)	C(6)–C(7)–C(2)	121·7 (8)
O(1)–P–C(14)	103·2 (3)	N–C(8)–C(9)	120·0 (6)
O(2)–P–N	112·5 (3)	N–C(8)–C(13)	119·7 (6)
O(2)–P–C(14)	117·1 (3)	C(9)–C(8)–C(13)	120·3 (7)
N–P–C(14)	106·4 (3)	C(8)–C(9)–C(10)	119·9 (7)
P–N–C(1)	124·2 (5)	C(9)–C(10)–C(11)	119·6 (7)
P–N–C(8)	113·4 (5)	C(10)–C(11)–C(12)	120·4 (8)
C(1)–N–C(8)	121·4 (6)	C(11)–C(12)–C(13)	120·5 (8)
N–C(1)–C(2)	115·9 (6)	C(12)–C(13)–C(8)	119·4 (7)
N–C(1)–S	121·2 (5)	P–C(14)–C(15)	120·4 (5)
C(2)–C(1)–S	122·9 (6)	P–C(14)–C(19)	120·8 (5)
C(1)–C(2)–C(3)	123·1 (7)	C(15)–C(14)–C(19)	118·9 (7)
C(1)–C(2)–C(7)	120·6 (7)	C(14)–C(15)–C(16)	121·6 (7)
C(3)–C(2)–C(7)	116·3 (7)	C(15)–C(16)–C(17)	119·4 (7)
C(2)–C(3)–O(1)	120·7 (7)	C(16)–C(17)–C(18)	119·4 (7)
C(2)–C(3)–C(4)	123·4 (7)	C(16)–C(17)–O(3)	124·3 (7)
O(1)–C(3)–C(4)	115·9 (7)	C(18)–C(17)–O(3)	116·3 (7)
C(3)–O(1)–P	119·6 (4)	C(17)–C(18)–C(19)	120·8 (7)
C(3)–C(4)–C(5)	118·0 (8)	C(18)–C(19)–C(14)	119·9 (7)
C(4)–C(5)–C(6)	120·0 (8)	C(17)–O(3)–C(20)	118·9 (6)

Discussion. Scheibye, Pedersen & Lawesson (1978*a*,*b*) showed that salicylanilide reacts with the dimer of *p*-methoxyphenylthioxophosphine sulphide to give the corresponding thioamide (yield 51%), but in addition two P-containing heterocyclic systems were isolated namely $C_{20}H_{16}NO_3PS$ (yield 21%, m.p. 173 °C) and $C_{20}H_{16}NO_2PS_2$ (yield 8%, m.p. 149 °C).

It was not possible to determine the structures of these P-containing heterocyclic compounds on the basis of analytical and spectral data and therefore the molecular structure of $C_{20}H_{16}NO_3PS$ was established by X-ray diffraction analysis.

Fig. 1 is a stereoscopic drawing of the molecule showing the numbering of the atoms. Bond distances are given in Table 2, and angles in Table 3.

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33796 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.