

1117  
MW

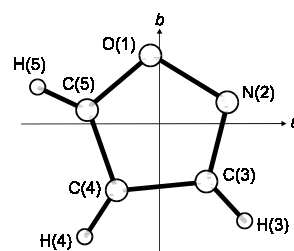
**C<sub>3</sub>H<sub>3</sub>NO**

**Isoxazole**

**C<sub>s</sub>**

$r_s$	Å <sup>a)</sup>	$\theta_s$	deg <sup>a)</sup>
O(1)–N(2)	1.3995(10)	C(5)–O(1)–C(2)	108.82(20)
N(2)=C(3)	1.3132(4)	O(1)–N(2)=C(3)	105.36(20)
C(3)–C(4)	1.4260(6)	N(2)=C(3)–C(4)	112.22(20)
C(4)=C(5)	1.3598(6)	C(3)–C(4)=C(5)	103.06(20)
C(5)–O(1)	1.3457(8)	C(4)=C(5)–O(1)	110.54(20)
C(3)–H(3)	1.0751(16)	C(4)–C(3)–H(3)	129.09(25)
C(4)–H(4)	1.0720(16)	C(3)–C(4)–H(4)	128.46(40)
C(5)–H(5)	1.0728(12)	C(4)=C(5)–H(5)	133.40(50)

Atom	$a_s$ [Å]	$b_s$ [Å]
O(1)	–0.0947	–1.1066
N(2)	1.1079	0.3909
C(3)	0.7593	–0.8752
C(4)	–0.6566	–1.0448
C(5)	–1.1191	0.2340
H(3)	1.5316	–1.6231
H(4)	–1.2188	–1.9576
H(5)	–2.1028	0.6619



<sup>a)</sup> Uncertainties are slightly larger than those of the original data.

Stiefvater, O.L.: J. Chem. Phys. **63** (1975) 2560.