

1600  $\text{C}_4\text{H}_5\text{NO}$   
MW

2-Methyloxazole

$\text{C}_s$

$r_0$	$\text{\AA}^{\text{a)}}$	$\theta_0$	deg
C(2)–O	1.358 <sup>b)</sup>	C(2)–O–C(5)	103.9 <sup>b)</sup>
O–C(5)	1.375 <sup>b)</sup>	O–C(5)=C(4)	108.0 <sup>b)</sup>
C(5)=C(4)	1.354 <sup>b)</sup>	C(5)=C(4)–N	109.1 <sup>b)</sup>
C(4)–N	1.397 <sup>b)</sup>	C(4)–N=C(2)	104.0 <sup>b)</sup>
N=C(2)	1.293 <sup>b)</sup>	N=C(2)–O	115.0 <sup>b)</sup>
C(2)–C (I)	1.5018(50) <sup>c)</sup>	C–C(2)–O (I)	116.7 <sup>b) c)</sup>
C(2)–C (II)	1.5146(50) <sup>c)</sup>	C–C(2)–O (II)	111.0 <sup>b) c)</sup>

<sup>a)</sup> Uncertainties were not estimated in the original paper.

<sup>b)</sup> Assumed.

<sup>c)</sup> The C(2)–C(methyl) bond was assumed to coincide with the  $\text{CH}_3$  internal rotation axis. Their distances (I) and (II) were derived from assumptions for the angles (I) and (II), respectively.

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