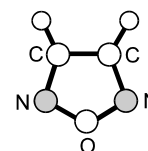


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MW**C₂H₂N₂O****Furazan**

1,2,5-Oxadiazole

1-Oxa-2,5-diazacyclopentadiene

C_{2v}

r_z	Å
O–N	1.3756(10)
N=C	1.3084(10)
C–C	1.4237(20)
C–H	1.0732(10)

θ_z	deg
N–O–N	111.30(7)
O–N=C	105.45(6)
N=C–C	108.90(5)
N=C–H	120.88(8)
C–C–H	130.22(3)

r_e^a	Å
O–N	1.3677(30)
N=C	1.3044(20)
C–C	1.4183(30)
C–H	1.0729(10)

θ_e^a	deg
N–O–N	111.30(7)
O–N=C	105.45(6)
N=C–C	108.90(5)
N=C–H	120.88(8)
C–C–H	130.22(3)

r_0	Å
O–N	1.3748(43)
N=C	1.3067(48)
C–C	1.4246(93)
C–H	1.0734(35)

θ_0	deg
N–O–N	111.22(45)
O–N=C	105.54(38)
N=C–C	108.85(31)
N=C–H	120.97(49)
C–C–H	130.17(21)

r_s^b	Å
O–N	1.3735(6)
N=C	1.3039(11)
C–C	1.4212(15)
C–H	1.0759(9)

θ_s^b	deg
N–O–N	111.16(7)
O–N=C	105.52(5)
N=C–C	108.90(4)
N=C–H	120.91(7)
C–C–H	130.18(3)

$r_m^{(1) c)}$	Å
O–N	1.3715(9)
N=C	1.3021(16)
C–C	1.4191(19)
C–H	1.0744(6)

$\theta_m^{(1) c)}$	deg
N–O–N	111.17(7)
O–N=C	105.51(5)
N=C–C	108.90(5)
N=C–H	120.91(7)
C–C–H	130.19(3)

$r_m^{(2) d)}$	Å
O–N	1.3709(13)
N=C	1.3017(17)
C–C	1.4210(22)
C–H	1.0760(16)

$\theta_m^{(2) d)}$	deg
N–O–N	111.17(8)
O–N=C	105.57(6)
N=C–C	108.84(6)
N=C–H	120.91(9)
C–C–H	130.24(6)

Structural parameters with the Laurie correction: $r(\text{C–D}) - r(\text{C–H})$ values were also given in the original paper.

^{a)} Extrapolated from r_z or θ_z .

^{b)} $\varepsilon_a = 0.149(38)$, $\varepsilon_b = 0.148(38)$, $\varepsilon_c = 0.368(77)$, in $\text{u } \text{\AA}^2$, included in the fit.

^{c)} $c_a = 0.041(11)$, $c_b = 0.041(11)$, $c_c = 0.065(15)$, in $\text{u}^{1/2} \text{\AA}$, included in the fit.

^{d)} $c_a = 0.052(30)$, $c_b = 0.063(18)$, $c_c = 0.094(30)$, in $\text{u}^{1/2} \text{\AA}$ and $d_a = -0.034(73)$,
 $d_b = -0.085(49)$, $d_c = -0.146(104)$, in $\text{u}^{1/2} \text{\AA}^2$, included in the fit.

Vázquez, J., Demaison, J., López-González, J.J., Boggs, J.E., Rudolph, H.D.: J. Mol. Spectrosc. **207** (2001) 224.

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