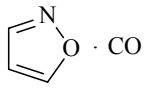
503 **$C_4H_3NO_2$** **Isoxazole – carbon monoxide (1/1)** **C_s**
MW (weakly bound complex) (effective symmetry class)
(large-amplitude motion)

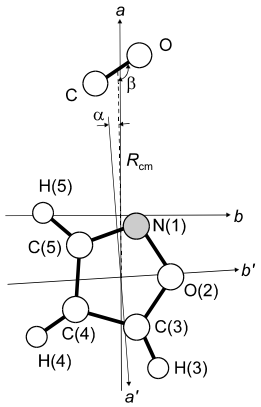


r_0	Å [a])	θ_0	deg [a])
R_{cm}	4.528(5)	α [b])	2.7(5)
C≡O	1.118(2)	β [c])	115.5(5)

Atom	a_0 [Å]	b_0 [Å]
N(1)	–0.2115	0.3372
O(2)	–1.3713	1.1173
C(3)	–2.4426	0.3089
C(4)	–2.0540	–0.9874
C(5)	–0.6312	–0.8984
H(3)	–3.4015	0.7910
H(4)	–2.6681	–1.8660
H(5)	0.0993	–1.6887
^{13}C[d])	2.8510	–0.5470
^{16}O[d])	3.4619	0.3894

The complex is planar, with CO lying approximately radially away from nitrogen in the isoxazole ring.

[a]) Uncertainties were not estimated in the original paper.
[b]) Angle between R_{cm} and the a' axis.
[c]) Angle between R_{cm} and the molecular axis of the carbon monoxide molecule.
[d]) Carbon and oxygen atoms of the $^{13}C^{16}O$ molecule.



The principal inertial axis system of the complex is denoted by a and b, and that of isoxazole by a' and b'.

McGlone, S., Bauder, A.: J. Chem. Phys. **109** (1998) 5383.