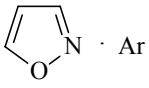
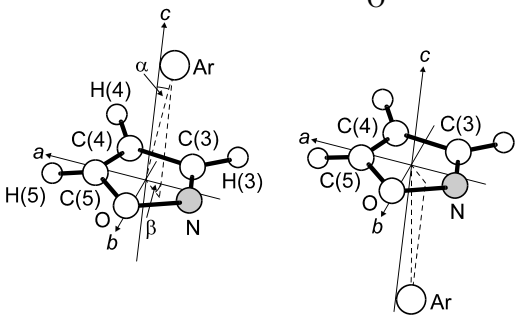
350 **C_3H_3ArNO** **Isoxazole – argon (1/1)** **C_1**
MW (weakly bound complex) (large-amplitude motion)

r_0	Å [a])
R [b])	3.44(1)

θ_0	deg [a])
α [c])	11.62(100)
β [d])	46.51(100)



Atom [e])	a_0 [Å]	b_0 [Å]	c_0 [Å]
N	–1.1069	0.3902	0.0
O	0.0958	1.1047	0.0
C(5)	1.1173	0.2322	0.0
C(4)	0.6554	–1.0428	0.0
C(3)	–0.7589	–0.8721	0.0
H(5)	2.1033	0.6604	0.0
H(4)	1.2181	–1.9578	0.0
H(3)	–1.5336	–1.6210	0.0
Ar	0.4875	0.5139	±3.4488



Enantiomers.

[a]) Uncertainties were not estimated in the original paper.
[b]) Distance between Ar and the ring plane.
[c]) Angle which the line from Ar to the center of mass (cm) of isoxazole encloses with the principal *c* axis of isoxazole.
[d]) Angle which the projection of the line from Ar to the cm of isoxazole on the molecular plane encloses with the principal *a* axis of izoxazole.
[e]) In the principal axis system of isoxazole.

Spoerel, U., Dreizler, H., Stahl, W., Kraka, E., Cremer, D.: J. Phys. Chem. **100** (1996) 14298.