

1082
MW

C₃H₃ArNS

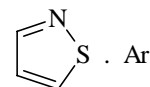
Isothiazole – argon (1/1)
(weakly bound complex)

C₁

Structure A

r_0	Å ^{a)}
R_{cm}	3.59(1)

θ_0	deg ^{a)}
Ar...cm...x ^{b)}	95.76(50)
Ar...cm...y ^{b)}	82.82(50)



Structure D

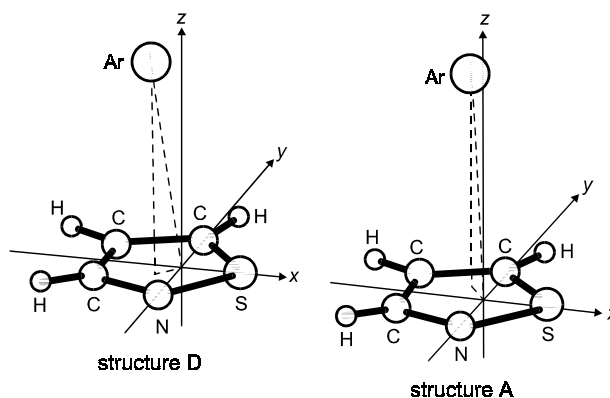
r_0	Å ^{a)}
R_{cm}	3.59(1)

θ_0	deg ^{a)}
Ar...cm...x ^{b)}	96.91(50)
Ar...cm...y ^{b)}	96.07(50)

An analysis of the ¹⁴N quadrupole coupling constants led to no unambiguous structure, except that the possible structure(s) are A and/or D. The structure of isothiazole was assumed to be unchanged by complexation.

^{a)} Uncertainties were not estimated in the original paper.

^{b)} The elevation angles of the argon atom above the *x* and *y* axes, respectively.



The two preferred structures

Kretschmer, U.: Ber. Bunsenges. Phys. Chem. **99** (1995) 891.