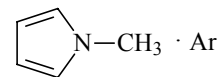


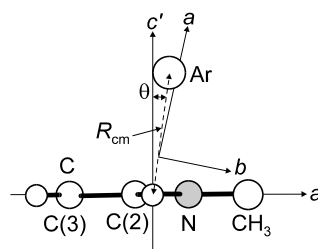
639  
MW $\text{C}_5\text{H}_7\text{ArN}$ *N*-Methyl-1*H*-pyrrole – argon (1/1)  
(weakly bound complex) $\text{G}_6$   
(effective symmetry class)  
(large-amplitude motion)

$r_0$	$\text{\AA}^{\text{a}}$	$\theta_0$	$\text{deg}^{\text{a}}$
$R_{\text{cm}}$	3.448(5)	$\theta^{\text{b}}$	5.46(50)



$r_s$	$\text{\AA}^{\text{a}}$
N–C(methyl)	1.451(3)
N...C(3)	2.226(3)
C(3)–C(4)	1.414(3)

Atom	$a_s [\text{\AA}]$	$b_s [\text{\AA}]$	$c_s [\text{\AA}]$
N	–1.0388	0.7256	0.0
C(2,5)	–1.1317	<sup>c)</sup>	$\pm 1.1201$
C(3,4)	–1.3169	–1.3670	$\pm 0.7070$
C(methyl)	–0.8023	2.15731	0.0



All rotational transitions were found to be split into A–E doublets because of the internal rotation of the methyl group. The potential barrier was determined to be  $V_3 = -32.11997 \text{ cm}^{-1}$  when  $V_6$  was assumed to be  $67.8021 \text{ cm}^{-1}$ , a value of the *N*-methylpyrrole monomer. The derived moments of inertia of the complex and its isotopomers led to a structure where argon is located above the aromatic ring plane. The substitution structure of the aromatic ring was shown to coincide almost exactly with that of the *N*-methylpyrrole monomer. The rotational spectra of the complex with a partially deuterated methyl group led to a staggered conformation with one of the C–H bonds perpendicular to the ring plane. The intermolecular stretching force constant is  $3.86 \text{ N m}^{-1}$ .

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

<sup>b)</sup> See figure for the definition, where  $a'$  and  $c'$  are the principal axes of the methylpyrrole.

<sup>c)</sup> Imaginary value; the actual coordinate will be very close to zero.

Huber, S., Makarewicz, J., Bauder, A.: Mol. Phys. **95** (1998) 1021.