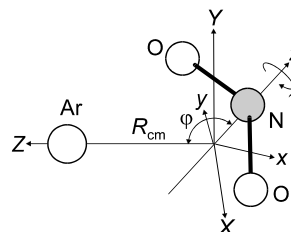


33  
MW, IR**ArNO<sub>2</sub>****Argon – nitrogen dioxide (1/1)**  
(weakly bound complex)**C<sub>s</sub>**  
(effective symmetry class)  
(large-amplitude motion)  
Ar · NO<sub>2</sub>

$r_0$	$\text{\AA}^a)$	$\theta_0$	$\text{deg}^a)$
$R_{\text{cm}}$	3.49042(5)	$\varphi^b)$	130.7(1) <sup>c)</sup>
		$\tau^b)$	10.1(1)

Changes in molecular parameters upon complexation can be caused by a geometric effect due to the rotation of the inertial axes from the monomer to the complex, and an electronic effect caused by a distortion of the electronic wave functions on complex formation. The electronic changes are shown to be very small. The absence of odd  $K_a$  states in the ground state was rationalized in terms of a high frequency tunneling motion of the NO<sub>2</sub> within the complex. Both a dynamics calculation and a model potential based on atom–atom interactions provided additional support for a nonplanar equilibrium structure with a low barrier to planarity.



The  $x, y, z$  axes represent the free NO<sub>2</sub> principal inertial axes ( $c, a, b$ ), and the  $X, Y, Z$  axes correspond to the complex inertial axes ( $B, C, A$ ).

<sup>a)</sup> Estimated standard errors.

<sup>b)</sup> See figure for the definition;  $\tau = 0$  when the Ar atom lies in the  $\sigma_v$  plane of the NO<sub>2</sub> monomer.

<sup>c)</sup> A value  $180^\circ - \varphi$  is equally valid from the analysis.

Low, R.J., Brooks, M.D., Whitham, C.J., Howard, B.J.: J. Chem. Phys. **105** (1996) 6756.

Replaces [II/25A\(2, 37\)](#)