

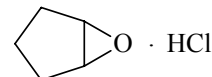
652  
MW $C_3H_7ClO$ **6-Oxabicyclo[3.1.0]hexane – hydrogen chloride (1/1)**

(weakly bound complex)

 $C_s$ (effective symmetry class)  
(large-amplitude motion)

$r_s$	$\text{\AA}^a$
O–C( $\alpha$ )	1.4391(14)
C( $\alpha$ )–C( $\beta$ )	1.50789(16)
C( $\beta$ )–C( $\gamma$ )	1.54523(17)

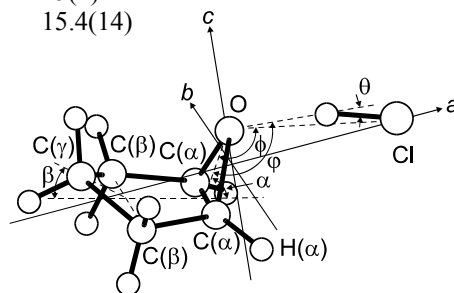
$\theta_s$	deg <sup>a</sup>
C( $\alpha$ )–O–C( $\alpha$ )	61.096(7)
C( $\beta$ )–C( $\gamma$ )–C( $\beta$ )	105.285(16)
$\alpha^a$	73.902(11)
$\beta^a$	29.02(4)



$r_0$	$\text{\AA}^a$
O–C( $\alpha$ )	1.432(6)
C( $\alpha$ )–C( $\beta$ )	1.515(6)
C( $\beta$ )–C( $\gamma$ )	1.546(6)
O...Cl	3.03(3)
O...H	1.77(4)
Cl...H( $\alpha$ )	3.43(7)

$\theta_0$	deg <sup>a</sup>
C( $\alpha$ )–O–C( $\alpha$ )	61.0(4)
C( $\beta$ )–C( $\gamma$ )–C( $\beta$ )	105.3(6)
$\alpha^b$	73.7(3)
$\beta^b$	29.4(7)
$\phi^b$	109(3)
$\varphi^b$	115(4)
$\theta^b$	15.4(14)

The derived structure of the complex has  $C_s$  symmetry with the hydrogen chloride pointing to the domain of the equatorial lone pair of electrons at the oxygen atom. The three atoms involved in the hydrogen bond adopt a bent arrangement,  $15.4(14)^\circ$  deviation from the linearity.



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

<sup>b</sup>) See figure for the definition.

Antolínez, S., Lesarri, A., López, J.C., Alonso, J.L.: Chem. Eur. J. **6** (2000) 3345.