

63  
MW

**CHBrClN**
**Hydrogen cyanide – bromine chloride (1/1)**

(weakly bound complex)

 $C_{\infty v}$ 

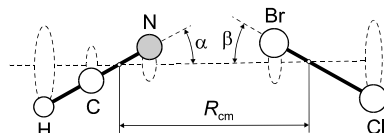
(effective symmetry class)

(large-amplitude motion)

 $H-C\equiv N \cdot BrCl$ 

Isotopic species	$r_s(R_{cm})$ [Å] <sup>a)</sup>	$r_s(N\cdots Br)$ [Å] <sup>a)</sup>	$k_\sigma$ [N m <sup>-1</sup> ]
$HC^{15}N \cdot {}^{79}Br^{35}Cl$	4.066(5)	2.834(5)	11.17
$HC^{15}N \cdot {}^{81}Br^{35}Cl$	4.055(5)	2.834(5)	10.93
$HC^{15}N \cdot {}^{79}Br^{37}Cl$	4.092(5)	2.835(5)	11.21
$HC^{15}N \cdot {}^{81}Br^{37}Cl$	4.081(5)	2.835(5)	11.03

Atom	$z_s$ [Å]
N	2.688
Br	-0.105
Cl	-2.383


<sup>a)</sup> Estimated assuming  $\alpha_{av} = 13.2(20)^\circ$  and  $\beta_{av} = 6.6(20)^\circ$ .

 Hinds, K., Legon, A.C.: Chem. Phys. Lett. **240** (1995) 467.