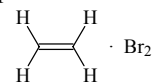
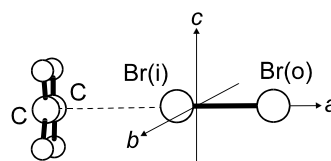


254
MW $\text{C}_2\text{H}_4\text{Br}_2$ **Ethene – dibromine (1/1)**
(weakly bound complex) C_{2v}
(effective symmetry class)
(large-amplitude motion)

$r_0^{\text{a})}$	$\text{C}_2\text{H}_4 \cdot {}^{79}\text{Br}^{79}\text{Br}$	$\text{C}_2\text{H}_4 \cdot {}^{81}\text{Br}^{79}\text{Br}$	$\text{C}_2\text{H}_4 \cdot {}^{79}\text{Br}^{81}\text{Br}$	$\text{C}_2\text{H}_4 \cdot {}^{81}\text{Br}^{81}\text{Br}$
$R_{\text{cm}} [\text{\AA}]$	4.2100(8)	4.1958(8)	4.1958(8)	4.2103(8)
$(*)\dots\text{Br}(\text{i}) [\text{\AA}]$	3.0684(8)	3.0685(8)	3.0677(8)	3.0687(8)

In the complex the Br_2 internuclear axis lies along the C_2 axis of C_2H_4 that is perpendicular to the plane of the C and H nuclei, so that Br(i) interacts with the center (*) of the π bond of ethene. The intermolecular van der Waals stretching force constant $k_\sigma = 8.8 \text{ N m}^{-1}$.

^{a)} Averages of the two sets of values derived using I_b and I_c are listed.



Legon, A.C., Thumwood, J.M.A.: Phys. Chem. Chem. Phys. **3** (2001) 1397.