

65  
MW**CHBrOS****Carbonyl sulfide – hydrogen bromide (1/1)**  
(weakly bound complex)**C<sub>∞v</sub>**  
(effective symmetry class)  
(large-amplitude motion)  
O=C=S · HBr

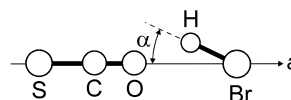
Isotopic species	$r_0(R_{\text{cm}})$ [Å] <sup>a)</sup>	$r_0(\text{O}\cdots\text{H})$ [Å] <sup>a)</sup>	$\theta_0(\alpha)$ [deg] <sup>a) b)</sup>	$k_\sigma$ <sup>c)</sup> [N m <sup>-1</sup> ]
OCS · H <sup>79</sup> Br	5.2633(20)	2.3853(20)	25.24(50)	0.485
OCS · H <sup>81</sup> Br	5.2639(20)	2.3855(20)	25.24(50)	0.492
OCS · D <sup>79</sup> Br	5.2477(20)	2.3471(20)	22.62(50)	0.612
OCS · D <sup>81</sup> Br	5.2487(20)	2.3472(20)	22.61(50)	0.614
OC <sup>34</sup> S · H <sup>79</sup> Br	5.2967(20)	2.3859(20)	25.28(50)	0.504

The complex is hydrogen bound and quasilinear with SCO...HBr atomic ordering.

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

<sup>b)</sup> Effective angle between the  $a$  inertial axis of the complex and the H–Br axis. It is essentially the O...Br–H angle.

<sup>c)</sup> Intermolecular stretching force constant.



Walker, A.R.H., Chen, W., Novick, S.E., Bean, B.D., Marshall, M.D.: J. Chem. Phys. **102** (1995) 7298.