

596  
MW $\text{C}_4\text{H}_{10}\text{OS}$ **Tetrahydrothiophene – water (1/1)**  
(weakly bound complex) $\text{C}_s$   
(effective symmetry class)  
(large-amplitude motion)

$r_0$	$\text{\AA}$	$\theta_0$	deg
S...H	2.37(4)	$\varphi^a$	85(3)
		$\beta^a$	162(12)

Atom	$ a_s  [\text{\AA}]$	$ b_s  [\text{\AA}]$	$ c_s  [\text{\AA}]$
S	0.0	1.2305	0.162

The rotational parameters were interpreted in terms of a geometry in which the water molecule acts as a proton donor lying close to the plane bisector to the CSC angle of tetrahydrothiophene. The “free” hydrogen is *entgegen* to the ring.

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

Sanz, M.E., López, J.C., Alonso, J.L., Maris, A., Favero, P.G., Caminati, W.: J. Phys. Chem. A **103** (1999) 5285.

