Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2020

Sulfur Hydrogen Bonding and Internal Dynamics in the Monohydrates of Thenyl Mercaptan and Thenyl Alcohol

Marcos Juanes,[a] Rizalina Tama Saragi,[a] Ruth Pinacho,[b] José E. Rubio,[b] Alberto Lesarri,*[a]

---

[a] Departamento de Química Física y Química Inorgánica and I.U. CINQUIMA, Facultad de Ciencias, Universidad de Valladolid, 47011 Valladolid (Spain), E-mail: alberto.lesarri@uva.es

[b] Departamento de Electrónica, Escuela de Ingeniería de Telecomunicaciones, Universidad de Valladolid 47011, Valladolid (Spain)

TABLE OF CONTENTS

Supplementary Figures

Figure S1. Predicted Gibbs energies (B3LYP-D3(BJ), kJ mol^{-1}) for the lowest-lying conformations of thenyl mercaptan (TM) and thenyl alcohol (TA), as collected in Tables S3 and S4. Molecular conformations are labeled according to the O-C-C-S/O (τ_1) and C-C-S/O-H (τ_2) dihedrals (G=+gauche, G'=-gauche T=trans).

Figure S2. Predicted interconversion barriers (B3LYP-D3(BJ)/def2-TZVP) for the internal rotation of the terminal hydrogen atom in the thiol/alcohol group of thenyl mercaptan (TM, blue trace) and thenyl alcohol (TA, red trace). The exocyclic sulfur/oxygen atom was kept fixed to the O-C-C-S/O gauche position. The barrier for the GG-GG´conversion in thenyl alcohol is 2.1 kJ mol^{-1}, ca. 1.9 kJ mol^{-1} smaller than in thenyl mercaptan.

Figure S3. Predicted geometry for conformer GG-Wa of the thenyl alcohol monohydrate TA···H_2O (B3LYP-D3(BJ)/def2-TZVP). The 3D figure is rotatable in the pdf file.

Figure S4. Predicted geometry for conformer GG´-Wdπ of the thenyl mercaptan monohydrate TM···H_2O (B3LYP-D3(BJ)/def2-TZVP). The 3D figure is rotatable in the pdf file.

Figure S5. Plot of the reduced electronic density gradient $s\left(=\frac{1}{1(3\pi^2)^{1/3}}\frac{|\nabla\rho|}{\rho^{4/3}}\right)$ versus the signed electronic density (= sign (λ2) ρ) for a) thenyl alcohol···water (upper panel, blue), b) thenyl mercaptan···water (lower panel). The plot minima at negative horizontal coordinates suggest attractive forces in the alcohol, much weaker in the mercaptan. Additionally, repulsive forces (positive horizontal coordinates) are indicative of weak forces and ring critical points.

Supplementary Tables

Table S1. DFT predictions for the optimized structure of thenyl mercaptan GG in the principal inertial axis system (B3LYP-D3(BJ) and MN15-L, basis set def2TZVP).

Table S2. DFT predictions for the optimized structure of thenyl alcohol GG in the principal inertial axis system (B3LYP-D3(BJ) and MN15-L, basis set def2TZVP).

Table S3. DFT predictions (B3LYP-D3(BJ) and MN15-L, basis set def2TZVP) for the most stable conformations of thenyl mercaptan.

Table S4. DFT predictions (B3LYP-D3(BJ) and MN15-L, basis set def2TZVP) for the most stable conformations of thenyl alcohol.

Table S5. Rotational parameters for conformer GG of thenyl mercaptan, including the parent species and all ^{13}C and the two ^{34}S monosubstituted species in natural abundance.

Table S6. Rotational parameters for conformer GG of thenyl alcohol, including the parent species and all ^{13}C and the ^{34}S monosubstituted species in natural abundance.

Table S7. Measured rotational transitions of thenyl mercaptan (conformer GG, parent isotopologue), residuals according to fit of Table S5 and assumed experimental uncertainties (all values in MHz).

Table S8. Measured rotational transitions of thenyl mercaptan (conformer GG, ^{34}S(1) isotopologue), residuals according to fit of Table S5 and assumed experimental uncertainties (all values in MHz).

Table S9. Measured rotational transitions of thenyl mercaptan (conformer GG, ^{13}C(2) isotopologue), residuals according to fit of Table S5 and assumed experimental uncertainties (all values in MHz).

Table S10. Measured rotational transitions of thenyl mercaptan (conformer GG, ^{13}C(3) isotopologue), residuals according to fit of Table S5 and assumed experimental uncertainties (all values in MHz).

Table S11. Measured rotational transitions of thenyl mercaptan (conformer GG, ^{13}C(4) isotopologue), residuals according to fit of Table S5 and assumed experimental uncertainties (all values in MHz).

Table S12. Measured rotational transitions of thenyl mercaptan (conformer GG, ^{13}C(5) isotopologue), residuals according to fit of Table S5 and assumed experimental uncertainties (all values in MHz).

Table S13. Measured rotational transitions of thenyl mercaptan (conformer GG, ^{13}C(6) isotopologue), residuals according to fit of Table S5 and assumed experimental uncertainties (all values in MHz).

Table S14. Measured rotational transitions of thenyl mercaptan (conformer GG, ^{34}S(7) isotopologue), residuals according to fit of Table S5 and assumed experimental uncertainties (all values in MHz).

Table S15. Measured rotational transitions of thenyl alcohol (conformer GG, parent isotopologue), residuals according to fit of Table S6 and assumed experimental uncertainties (all values in MHz).

Table S16. Measured rotational transitions of thenyl alcohol (conformer GG, ^{34}S(1) isotopologue), and residuals according to fit of Table S6 and assumed experimental uncertainties (all values in MHz).

Table S17. Measured rotational transitions of thenyl alcohol (conformer GG, ^{13}C(2) isotopologue), residuals according to fit of Table S6 and assumed experimental uncertainties (all values in MHz).

Table S18. Measured rotational transitions of thenyl alcohol (conformer GG, ^{13}C(3) isotopologue), residuals according to fit of Table S6 and assumed experimental uncertainties (all values in MHz).

Table S19. Measured rotational transitions of thenyl alcohol (conformer GG, ^{13}C(4) isotopologue), residuals according to fit of Table S6 and assumed experimental uncertainties (all values in MHz).

Table S20. Measured rotational transitions of thenyl alcohol (conformer GG, ^{13}C(5) isotopologue), residuals according to fit of Table S6 and assumed experimental uncertainties (all values in MHz).

Table S21. Measured rotational transitions of thenyl alcohol (conformer GG, ^{13}C(6) isotopologue), residuals according to fit of Table S6 and assumed experimental uncertainties (all values in MHz).

Table S22. Results of the effective structure (r_0) determination for the thenyl mercaptan conformer GG. The fitted parameters are compared with the theoretical predictions (theory, B3LYP-D3(BJ)/def2TZVP).

Table S23. Differences with the experimental rotational constants for the fitted structure of the thenyl mercaptan conformer GG of Table S22.

Table S24. Results of the effective structure determination for the thenyl alcohol conformer GG. The fitted parameters (r_0) are compared with the theoretical predictions (theory, B3LYP- GD3BJ /def2TZVP).

Table S25. Differences with the experimental rotational constants for the fitted structure of the thenyl alcohol conformer GG of Table S24.

Table S26. Substitution coordinates for conformer GG of thenyl mercaptan (theoretical predictions in Table S1).

Table S27. Substitution coordinates for conformer GG of thenyl alcohol (theoretical predictions in Table S2).

Table S28. Analysis of the rotational spectrum of ^{34}S-thenyl alcohol···$H_2{}^{16}O$.

Table S29. Analysis of the rotational spectrum of thenyl alcohol···$H_2{}^{18}O$.

Table S30. Measured rotational transitions for isomer I of thenyl alcohol···$H_2{}^{16}O$, residuals according to fit of Table 3 and assumed experimental uncertainties (all values in MHz).

Table S31. Measured rotational transitions for isomer I of ^{34}S-thenyl alcohol···$H_2{}^{16}O$, residuals according to fit of Table S28 and assumed experimental uncertainties (all values in MHz).

Table S32. Measured rotational transitions for isomer I of thenyl alcohol···$H_2{}^{18}O$, residuals according to fit of Table S29 and assumed experimental uncertainties (all values in MHz).

Table S33. Analysis of the rotational spectrum of thenyl mercaptan···$H_2{}^{18}O$.

Table S34. Measured rotational transitions for isomer I of thenyl mercaptan···$H_2{}^{16}O$, residuals according to fit of Table 4 and assumed experimental uncertainties (all values in MHz).

Table S35. Measured rotational transitions for isomer I of thenyl mercaptan···$H_2{}^{18}O$, residuals according to fit of Table S31 and assumed experimental uncertainties (all values in MHz).

Table S36. B2PLYP-D3(BJ) and ωB97XD DFT predictions for the thenyl alcohol monohydrate TA···H_2O.

Table S37. Substitution coordinates for the oxygen atom and the ring sulfur in thenyl alcohol···H_2O using the Kraitchman equations (unsigned), and comparison with the DFT prediction (B3LYP- GD3BJ /def2TZVP).

Table S38. Results of the effective structure (r_0) determination for thenyl alcohol···H_2O. The fitted parameters are compared with the theoretical predictions (theory, B3LYP-GD3BJ /def2TZVP). The residuals of the fit of the experimental rotational constants are shown below.

Table S39. Equilibrium coordinates for thenyl alcohol···H_2O according to the DFT prediction (B3LYP- GD3BJ /def2TZVP).

Table S40. B2PLYP-D3(BJ) and ωB97XD DFT predictions for the thenyl mercaptan monohydrate TM···H_2O.

Table S41. Substitution coordinates for the oxygen atom in thenyl mercaptan···H_2O using the Kraitchman equations (unsigned), and comparison with the DFT prediction (B3LYP- GD3BJ /def2TZVP).

Table S42. Results of the effective structure determination for thenyl mercaptan···H_2O. The fitted parameters (r_0) are compared with the theoretical predictions (theory, B3LYP-GD3BJ /def2TZVP). The differences with the experimental rotational constants for the fitted structure are shown below.

Table S43. Equilibrium coordinates for thenyl mercaptan···H_2O according to the DFT prediction (B3LYP- GD3BJ /def2TZVP).

Figure S1. Predicted Gibbs energies (B3LYP-D3(BJ), kJ mol^{-1}) for the lowest-lying conformations of thenyl mercaptan (TM) and thenyl alcohol (TA), as collected in Tables S3 and S4. Molecular conformations are labeled according to the O-C-C-S/O (τ_1) and C-C-S/O-H (τ_2) dihedrals (G=+gauche, G'=-gauche T=trans).

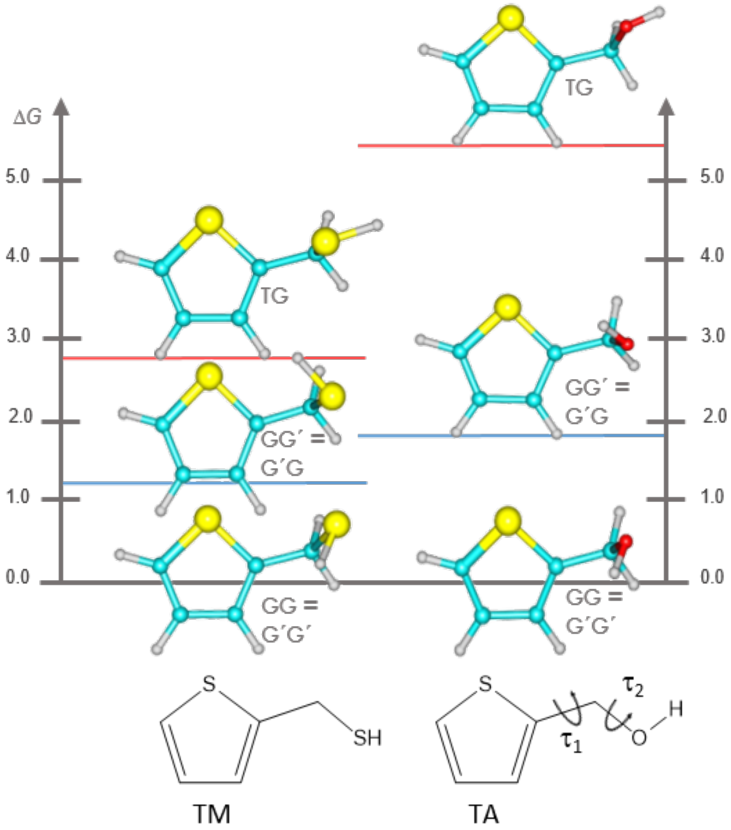


Figure S2. Predicted interconversion barriers (B3LYP-D3(BJ)/def2-TZVP) for the internal rotation of the terminal hydrogen atom in the thiol/alcohol group of thenyl mercaptan (TM, blue trace) and thenyl alcohol (TA, red trace). The exocyclic sulfur/oxygen atom was kept fixed to the O-C-C-S/O gauche position. The barrier for the GG-GG´conversion in thenyl alcohol is 2.1 kJ mol^{-1}, ca. 1.9 kJ mol^{-1} smaller than in thenyl mercaptan.

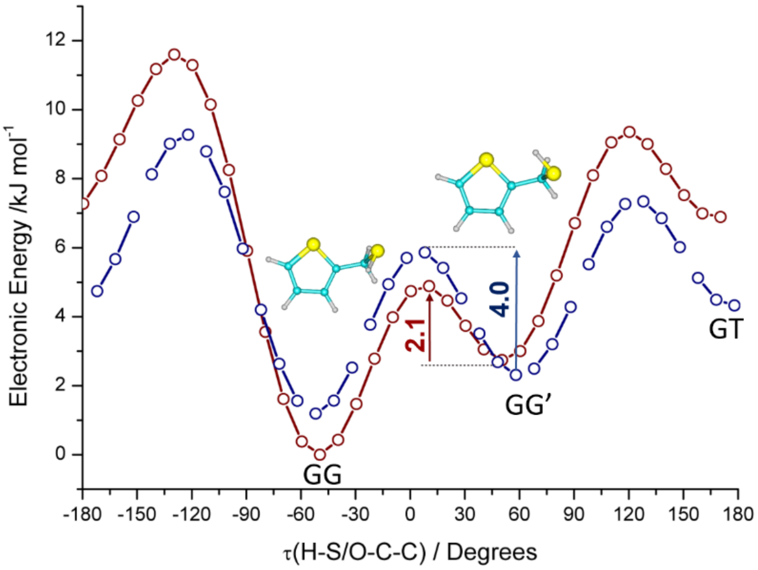


Figure S3. Predicted geometry for conformer GG-Wa of the thenyl alcohol monohydrate TA···H_2O (B3LYP-D3(BJ)/def2-TZVP). The 3D figure is rotatable in the pdf file.

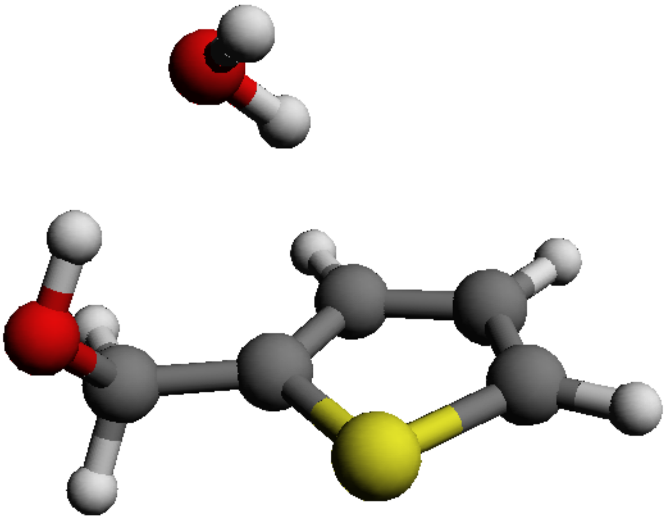


Figure S4. Predicted geometry for conformer GG´-Wdπ of the thenyl mercaptan monohydrate TM···H_2O (B3LYP-D3(BJ)/def2-TZVP). The 3D figure is rotatable in the pdf file.

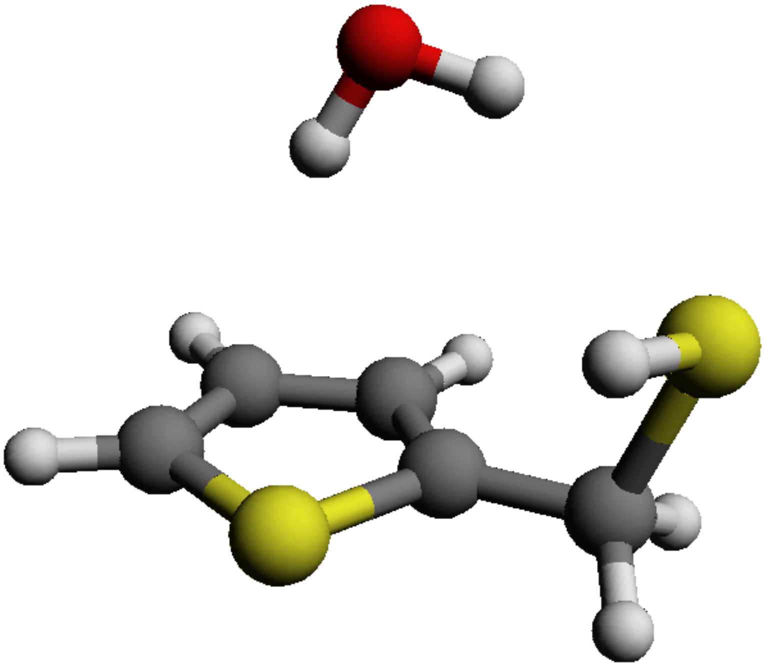
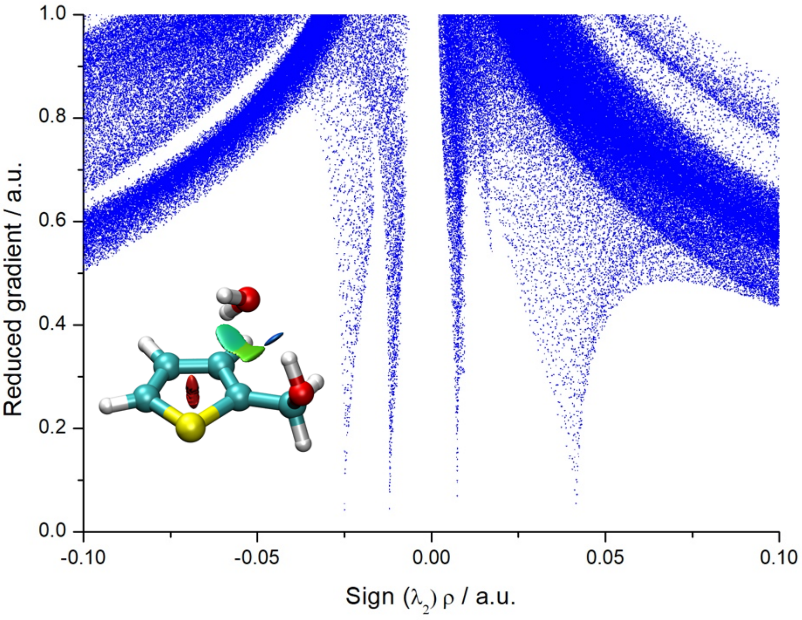


Figure S5. Plot of the reduced electronic density gradient $s\left(=\frac{1}{1(3\pi^2)^{1/3}}\frac{|\nabla\rho|}{\rho^{4/3}}\right)$ versus the signed electronic density (= sign ($\lambda2$) ρ) for a) thenyl alcohol···water (upper panel, blue), b) thenyl mercaptan···water (lower panel). The plot minima at negative horizontal coordinates suggest attractive forces in the alcohol, much weaker in the mercaptan. Additionally, repulsive forces (positive horizontal coordinates) are indicative of weak forces and ring critical points.



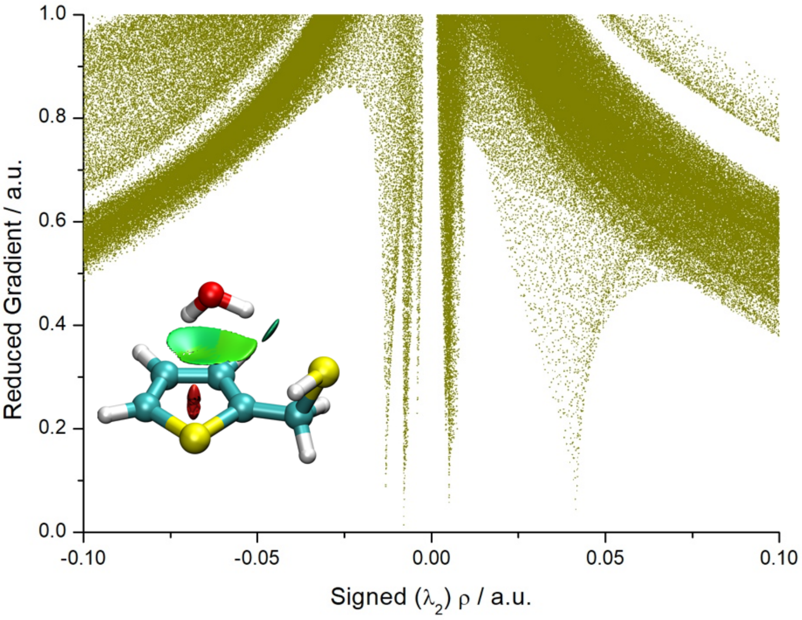
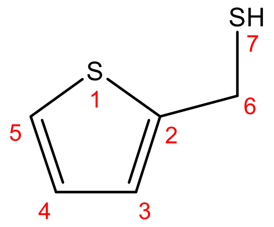


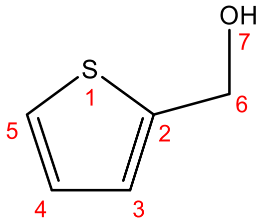
Table S1. DFT predictions for the optimized structure of thenyl mercaptan GG in the principal inertial axis system (B3LYP-D3(BJ) and MN15-L, basis set def2TZVP).



	Thenyl Mercaptan GG		
	a / Å[a]	***b*** / Å	***c*** / Å
S(1)	0.8751/ 0.7311[b]	-1.1360/-1.1008	-0.1822/-0.2049
C(2)	0.1011/ 0.1243	0.4014/ 0.5102	-0.3626/-0.2369
C(3)	0.9587/ 1.1207	1.4140/ 1.4110	-0.0290/ 0.0723
C(4)	2.2449/ 2.3803	0.9544/ 0.7865	0.3660/ 0.3209
C(5)	2.3455/ 2.3129	-0.4050/-0.5805	0.3275/ 0.1981
C(6)	-1.3104/-1.2969	0.5331/ 0.8282	-0.8106/-0.5978
S(7)	-2.5599/-2.5455	-0.1149/-0.1691	0.3775/ 0.2814
H(3)	3.1972/ 3.1072	-1.0174/-1.3108	0.5737/ 0.3440
H(4)	3.0547/ 3.2915	1.6046/ 1.3254	0.6635/ 0.5877
H(5)	0.6751/ 0.9457	2.4567/ 2.4894	-0.0701/ 0.1131
H(6)	-1.5023/-1.5002	-0.0329/ 0.6266	-1.7229/-1.6651
H(6’)	-1.5257/-1.4729	1.5794/ 1.9044	-1.0209/-0.4313
H(7)	-2.1258/-2.0745	0.5868/ 0.0610	1.4374/ 1.5237

[a] Principal inertial axes denoted *a*, *b*, *c*. [b] B3LYP-GD3 / MN15-L coordinates in Angstrom.

Table S2. DFT predictions for the optimized structure of thenyl alcohol GG in the principal inertial axis system (B3LYP-D3(BJ) and MN15-L, basis set def2TZVP).



Thenyl Alcohol GG			
	a / Å[a]	***b*** / Å	***c*** / Å
S(1)	0.4858/ 0.3974	-1.1377/-1.1157	-0.1240/-0.1298
C(2)	-0.3426/-0.3232	0.3794/ 0.4485	-0.2276/-0.1669
C(3)	0.5271/ 0.6300	1.4164/ 1.4260	-0.0273/ 0.0205
C(4)	1.8643/ 1.9464	0.9934/ 0.8984	0.2043/ 0.1836
C(5)	1.9897/ 1.9648	-0.3649/-0.4752	0.1810/ 0.1259
C(6)	-1.8115/-1.8020	0.45611/ 0.6160	-0.4869/-0.3900
O(7)	-2.5990/-2.5843	-0.1872/-0.2550	0.5131/ 0.4107
H(3)	2.8797/ 2.8177	-0.9527/-1.1427	0.3355/ 0.2398
H(4)	2.6902/ 2.8373	1.6661/ 1.5074	0.3839/ 0.3496
H(5)	0.2153/ 0.3833	2.4517/ 2.4910	-0.0501/ 0.0393
H(6)	-2.0768/-2.0799	-0.0434/ 0.3765	-1.4198/-1.4327
H(6’)	-2.0846/-2.0527	1.5131/ 1.6857	-0.5872/-0.2182
H(7)	-2.3043/-2.2638	0.1310/-0.1683	1.3743/ 1.3208

[a] Principal inertial axes denoted *a*, *b*, *c*. [b] B3LYP-GD3 / MN15-L coordinates in Angstrom.

Table S3. DFT predictions (B3LYP-D3(BJ) and MN15-L, basis set def2TZVP) for the most stable conformations of thenyl mercaptan.

	Theory[c,d]		
	GG	GG’	GT
A / MHz[a]	4163.33/4335.04	4077.68/4074.80	4095.10/4237.78
B / MHz	1131.97/1152.19	1116.17/1126.10	1143.90/1168.78
C / MHz	975.51/967.44	974.09/981.35	995.04/990.61
D_J / kHz	0.147/0.111	0.166/0.170	0.192/0.148
D_{JK} / kHz	4.667/2.837	3.093/6.212	6.980/3.271
D_K / kHz	0.296/2.465	-0.918/-3.011	-3.163/2.263
d_1 / kHz	-0.014/-0.020	-0.009/-0.007	-0.020/-0.018
d_2 / kHz	-0.002/-0.012	0.006/0.009	0.006/-0.012
$\|\mu_a\|$ / D	1.21/1.29	1.27/1.36	0.40/0.42
$\|\mu_b\|$ / D	1.22/1.28	0.09/0.22	0.79/1.26
$\|\mu_c\|$ / D	0.19/0.12	0.56/0.61	1.30/1.11
ΔE / kJ mol^{-1} [b]	0.0/0.0	1.10/2.10	3.26/3.86
ΔG / kJ mol^{-1}	0.0/0.0	1.21/0.70	2.72/3.30

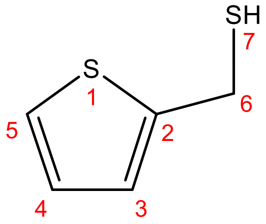
[a] Rotational constants (A, B, C), Watson’s S-reduction centrifugal distortion constants (D_J, D_{JK}, D_K, d_1, d_2) and electric dipole moments (μ_α, α = a, b, c). [b] Relative energies corrected with the zero-point energy (ZPE) and Gibbs energy (ΔG, 298K, 1 atm). [c] B3LYP-GD3BJ and MN15-L calculations, respectively (basis set def2TZVP). [d] Notation according to dihedrals τ_1(S-C-C-S/O) and τ_2(S-C-C-S/O): +gauche (G), -gauche (G’) and trans (T).

Table S4. DFT predictions (B3LYP-D3(BJ) and MN15-L, basis set def2TZVP) for the most stable conformations of thenyl alcohol.

	Theory[c,d]		
	GG	GG’	GT
A / MHz[a]	4619.71/4699.21	4528.70/4521.34	4694.52/4766.17
B / MHz	1728.88/1750.34	1696.59/1700.30	1744.64/1770.48
C / MHz	1349.57/1343.48	1347.55/1352.55	1348.01/1344.52
D_J / kHz	0.182/0.174	0.256/0.295	0.179/0.164
D_{JK} / kHz	5.033 /3.985	6.066/7.979	6.545/3.092
D_K / kHz	-2.377/-1.600	-4.694/-6.623	-3.480/-1.168
d_1 / kHz	-0.044/-0.065	-0.024/-0.036	0.070/-0.068
d_2 / kHz	-0.016/-0.029	0.014 /0.022	0.037/-0.029
$\|\mu_a\|$ / D	1.36/1.26	1.50/1.43	0.69/0.83
$\|\mu_b\|$ / D	1.43/1.27	0.27/0.15	0.93/1.13
$\|\mu_c\|$ / D	0.34/0.62	0.10/0.10	1.24/0.99
ΔE/kJmol^{-1} [b]	0.0/0.0	2.42/3.69	6.13/5.76
ΔG/kJmol^{-1}	0.0/0.0	1.91/2.64	5.63/5.85

[a]Rotational constants (A, B, C), Watson’s S-reduction centrifugal distortion constants (D_J, D_{JK}, D_K, d_1, d_2) and electric dipole moments (μ_α, α = a, b, c). [b]Relative energies corrected with the zero-point energy (ZPE) and Gibbs energy (ΔG, 298K, 1 atm). [c]B3LYP-GD3BJ and MN15-L calculations, respectively (basis set def2TZVP). [d]Notation according to dihedrals τ_1(S-C-C-S/O) and τ_2(S-C-C-S/O): +gauche (G), -gauche (G’) and trans (T).

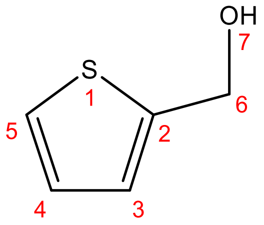
Table S5. Rotational parameters for conformer GG of thenyl mercaptan, including the parent species and all ^{13}C and the two ^{34}S monosubstituted species in natural abundance.



	Conformer GG							
	Parent	^{34}S(1)	^{13}C(2)	^{13}C(3)	^{13}C(4)	^{13}C(5)	^{13}C(6)	^{34}S(7)
A / MHz[a]	4209.1932(10)[c]	4121.7106(69)	4198.9898(23)	4177.154(10)	4140.4026(51)	4198.7318(58)	4175.794(11)	4199.9984(57)
B / MHz	1142.26901(51)	1138.6463(14)	1128.22130(88)	1128.6180(28)	1139.6868(14)	1142.0068(19)	1136.4519(41)	1109.7249(11)
C / MHz	976.51273(34)	969.3252(16)	965.99840(79)	965.2798(26)	970.8757(11)	976.2103(16)	972.6315(43)	952.9586(11)
D_J / kHz	0.1486(48)	[0.1486]	[0.1486]	[0.1486]	[0.1486]	[0.1486]	[0.1486]	[0.1486]
D_{JK} / kHz	6.4404(81)	[6.4404]	[6.4404]	[6.4404]	[6.4404]	[6.4404]	[6.4404]	[6.4404]
D_K / kHz	[0.][d]	[0.]	[0.]	[0.]	[0.]	[0.]	[0.]	[0.]
d_1 / kHz	-0.0190(28)	[-0.0190]	[-0.0190]	[-0.0190]	[-0.0190]	[-0.0190]	[-0.0190]	[-0.0190]
d_2 / kHz	-0.0093(14)	[-0.0093]	[-0.0093]	[-0.0093]	[-0.0093]	[-0.0093]	[-0.0093]	[-0.0093]
N[b]	40	17	9	9	7	9	8	19
σ / kHz	9.4	16.3	3.9	14.2	6.5	7.8	15.1	13.9

[a]Rotational constants (A, B, C), Watson's S-reduction centrifugal distortion constants (D_J, D_{JK}, D_K, d_1, d_2). [b]Number of transitions (N) and rms deviation (σ) of the fit. [c]Standard errors in parentheses in units of the last digit. [d]Values in square brackets were kept fixed in the fit.

Table S6. Rotational parameters for conformer GG of thenyl alcohol, including the parent species and all ^{13}C and the ^{34}S monosubstituted species in natural abundance.



	Conformer GG						
	Parent	^{34}S(1)	^{13}C(2)	^{13}C(3)	^{13}C(4)	^{13}C(5)	^{13}C(6)
A / MHz[a]	4617.0988(42)[c]	4512.1450(21)	4610.0423(68)	4575.6606(40)	4534.0769(69)	4608.9881(57)	4598.6068(48)
B / MHz	1730.4574(10)	1727.6426(10)	1707.3037(14)	1709.70515(85)	1728.8039(15)	1729.5741(11)	1710.0061(10)
C / MHz	1349.2861(10)	1338.6563(10)	1334.8124(15)	1333.4077(10)	1341.1004(17)	1348.4620(12)	1336.9243(12)
D_J / kHz	[0.][d]	[0.]	[0.]	[0.]	[0.]	[0.]	[0.]
D_{JK} / kHz	5.21(16)	[5.21]	[5.21]	[5.21]	[5.21]	[5.21]	[5.21]
D_K / kHz	[0.]	[0.]	[0.]	[0.]	[0.]	[0.]	[0.]
d_1 / kHz	-0.0515(88)	[-0.0515]	[-0.0515]	[-0.0515]	[-0.0515]	[-0.0515]	[-0.0515]
d_2 / kHz	-0.0154(42)	[-0.0154]	[-0.0154]	[-0.0154]	[-0.0154]	[-0.0154]	[-0.0154]
N[b]	29	18	11	11	10	11	10
σ / kHz	10.3	9.8	10.1	6.5	10.5	9.2	7.4

[a]Rotational constants (A, B, C), Watson's S-reduction centrifugal distortion constants (D_J, D_{JK}, D_K, d_1, d_2). [b]Number of transitions (N) and rms deviation (σ) of the fit. [c]Standard errors in parentheses in units of the last digit. [d]Values in square brackets were kept fixed in the fit.

Table S7. Measured rotational transitions of thenyl mercaptan (conformer GG, parent isotopologue), residuals according to fit of Table S5 and assumed experimental uncertainties (all values in MHz).

J'	K_{-1}'	K_{+1}'	J''	K_{-1}''	K_{+1}''	Frequency[1]	Residuals	Uncertainty
1	0	1	0	0	0	2118.7544	-0.0267	0.020
1	1	0	1	0	1	3232.6698	0.0022	0.020
2	1	1	2	0	2	3404.9392	0.0030	0.020
3	0	3	2	1	2	3422.5464	-0.0263	0.020
3	1	2	3	0	3	3675.4489	0.0017	0.020
4	1	3	4	0	4	4058.1226	0.0094	0.020
2	1	2	1	1	1	4071.7721	-0.0052	0.020
2	0	2	1	0	1	4231.0342	0.0142	0.020
2	1	1	1	1	0	4403.3079	0.0192	0.020
5	1	4	5	0	5	4569.9239	0.0263	0.020
6	1	5	5	2	4	4918.6587	-0.0007	0.020
1	1	1	0	0	0	5185.6995	0.0069	0.020
6	1	5	6	0	6	5228.5552	-0.0023	0.020
1	1	0	0	0	0	5351.4481	-0.0005	0.020
4	0	4	3	1	3	5729.2223	-0.0066	0.020
7	1	6	7	0	7	6049.3112	-0.0039	0.020
3	1	3	2	1	2	6103.6678	0.0187	0.020
3	0	3	2	0	2	6330.2517	0.0102	0.020
3	2	2	2	2	1	6356.1678	-0.0077	0.020
3	2	1	2	2	0	6382.2627	0.0012	0.020
3	1	2	2	1	1	6600.7495	-0.0029	0.020
8	1	7	8	0	8	7041.0728	-0.0011	0.020
2	1	2	1	0	1	7138.6933	0.0046	0.020
5	0	5	4	1	4	8064.3296	-0.0035	0.020
4	1	4	3	1	3	8130.9199	-0.0028	0.020
5	1	5	4	1	4	10152.4260	-0.0004	0.005
4	2	3	4	1	4	10289.3241	-0.0019	0.005
6	0	6	5	1	5	10406.0533	-0.0003	0.005
5	0	5	4	0	4	10466.0275	0.0005	0.005
5	3	3	4	3	2	10614.0828	0.0001	0.005
5	3	2	4	3	1	10617.4599	-0.0001	0.005
5	1	4	4	1	3	10977.8118	0.0004	0.005
6	1	6	5	1	5	12167.2760	0.0011	0.005
6	0	6	5	0	5	12494.1454	-0.0016	0.005
8	2	7	8	1	8	12531.7671	0.0001	0.005
6	5	2	5	5	1	12726.9881	-0.0011	0.005
6	5	1	5	5	0	12726.9881	-0.0017	0.005
7	0	7	6	1	6	12733.1093	0.0001	0.005
6	4	3	5	4	2	12733.5232	0.0019	0.005
6	4	2	5	4	1	12733.6403	0.0004	0.005
6	1	5	5	1	4	13152.8068	-0.0002	0.005

Table S8. Measured rotational transitions of thenyl mercaptan (conformer GG, ^{34}S(1) isotopologue), residuals according to fit of Table S5 and assumed experimental uncertainties (all values in MHz).

J'	K_{-1}'	K_{+1}'	J''	K_{-1}''	K_{+1}''	Frequency	Residuals	Uncertainty
1	0	1	0	0	0	2107.9421	-0.0289	0.020
1	1	0	1	0	1	3152.3824	0.0100	0.020
2	1	1	2	0	2	3328.6691	-0.0032	0.020
3	0	3	2	1	2	3475.2250	-0.0217	0.020
3	1	2	3	0	3	3606.0929	0.0104	0.020
4	1	3	4	0	4	3999.4240	-0.0169	0.020
2	1	2	1	1	1	4046.5951	0.0029	0.020
2	0	2	1	0	1	4208.9343	0.0010	0.020
2	1	1	1	1	0	4385.2448	0.0116	0.020
1	1	1	0	0	0	5091.0115	-0.0109	0.020
4	0	4	3	1	3	5772.1972	0.0330	0.020
3	1	3	2	1	2	6065.5594	-0.0298	0.020
3	0	3	2	0	2	6295.9552	-0.0019	0.020
3	2	2	2	2	1	6323.7429	-0.0021	0.020
3	2	1	2	2	0	6351.6855	0.0005	0.020
3	1	2	2	1	1	6573.3671	0.0000	0.020
2	1	2	1	0	1	7029.6645	0.0208	0.020

Table S9. Measured rotational transitions of thenyl mercaptan (conformer GG, ^{13}C(2) isotopologue), residuals according to fit of Table S5 and assumed experimental uncertainties (all values in MHz).

J'	K_{-1}'	K_{+1}'	J''	K_{-1}''	K_{+1}''	Frequency	Residuals	Uncertainty
1	1	0	1	0	1	3232.9798	0.0013	0.020
2	1	1	2	0	2	3401.4344	0.0004	0.020
2	0	2	1	0	1	4182.1718	-0.0037	0.020
2	1	1	1	1	0	4350.6265	-0.0045	0.020
1	1	1	0	0	0	5164.9690	-0.0057	0.020
3	1	3	2	1	2	6035.4352	0.0023	0.020
3	0	3	2	0	2	6257.6652	-0.0034	0.020
3	1	2	2	1	1	6521.9522	0.0058	0.020
2	1	2	1	0	1	7096.9462	0.0039	0.020

Table S10. Measured rotational transitions of thenyl mercaptan (conformer GG, ^{13}C(3) isotopologue), residuals according to fit of Table S5 and assumed experimental uncertainties (all values in MHz).

J'	K_{-1}'	K_{+1}'	J''	K_{-1}''	K_{+1}''	Frequency	Residuals	Uncertainty
1	1	0	1	0	1	3211.8797	0.0181	0.020
2	1	1	2	0	2	3381.5503	-0.0122	0.020
3	1	2	3	0	3	3647.9592	0.0124	0.020
2	0	2	1	0	1	4181.4089	0.0070	0.020
2	1	1	1	1	0	4351.1152	0.0124	0.020
1	1	1	0	0	0	5142.4026	-0.0182	0.020
3	1	3	2	1	2	6032.7291	0.0133	0.020
3	0	3	2	0	2	6256.1870	0.0014	0.020
3	1	2	2	1	1	6522.5482	-0.0216	0.020

Table S11. Measured rotational transitions of thenyl mercaptan (conformer GG, ^{13}C(4) isotopologue), residuals according to fit of Table S5 and assumed experimental uncertainties (all values in MHz).

J'	K_{-1}'	K_{+1}'	J''	K_{-1}''	K_{+1}''	Frequency	Residuals	Uncertainty
3	1	2	3	0	3	3621.6021	0.0050	0.020
2	0	2	1	0	1	4214.1914	-0.0050	0.020
1	1	1	0	0	0	5111.2652	0.0002	0.020
3	1	3	2	1	2	6074.1901	0.0137	0.020
3	0	3	2	0	2	6304.0495	-0.0035	0.020
3	1	2	2	1	1	6580.4243	-0.0034	0.020
2	1	2	1	0	1	7052.9819	-0.0052	0.020

Table S12. Measured rotational transitions of thenyl mercaptan (conformer GG, ^{13}C(5) isotopologue), residuals according to fit of Table S5 and assumed experimental uncertainties (all values in MHz).

J'	K_{-1}'	K_{+1}'	J''	K_{-1}''	K_{+1}''	Frequency	Residuals	Uncertainty
1	1	0	1	0	1	3222.5013	-0.0072	0.020
2	1	2	1	1	1	4070.6038	-0.0038	0.020
2	0	2	1	0	1	4229.8675	0.0012	0.020
2	1	1	1	1	0	4402.2083	0.0088	0.020
1	1	1	0	0	0	5174.9349	0.0062	0.020
3	1	3	2	1	2	6101.8705	-0.0094	0.020
3	0	3	2	0	2	6328.4636	0.0129	0.020
3	1	2	2	1	1	6599.0925	-0.0103	0.020
2	1	2	1	0	1	7127.3208	0.0009	0.020

Table S13. Measured rotational transitions of thenyl mercaptan (conformer GG, ^{13}C(6) isotopologue), residuals according to fit of Table S5 and assumed experimental uncertainties (all values in MHz).

J'	K_{-1}'	K_{+1}'	J''	K_{-1}''	K_{+1}''	Frequency	Residuals	Uncertainty
1	1	0	1	0	1	3203.1536	0.0037	0.020
2	1	2	1	1	1	4054.3437	0.0272	0.020
2	0	2	1	0	1	4211.7238	0.0071	0.020
2	1	1	1	1	0	4381.9427	-0.0133	0.020
1	1	1	0	0	0	5148.4227	0.0102	0.020
3	0	3	2	0	2	6301.4984	-0.0202	0.020
3	1	2	2	1	1	6568.8252	0.0119	0.020
2	1	2	1	0	1	7093.6322	-0.0138	0.020

Table S14. Measured rotational transitions of thenyl mercaptan (conformer GG, ^{34}S(7) isotopologue), residuals according to fit of Table S5 and assumed experimental uncertainties (all values in MHz).

J'	K_{-1}'	K_{+1}'	J''	K_{-1}''	K_{+1}''	Frequency	Residuals	Uncertainty
1	0	1	0	0	0	2062.7022	0.0191	0.020
3	0	3	2	1	2	3225.5292	-0.0180	0.020
1	1	0	1	0	1	3247.0107	-0.0160	0.020
2	1	1	2	0	2	3409.5645	-0.0165	0.020
3	1	2	3	0	3	3664.1955	0.0052	0.020
2	1	2	1	1	1	3968.5726	0.0016	0.020
4	1	3	4	0	4	4023.3016	0.0108	0.020
2	0	2	1	0	1	4119.5512	0.0030	0.020
2	1	1	1	1	0	4282.0811	-0.0213	0.020
1	1	1	0	0	0	5152.9408	-0.0028	0.020
4	0	4	3	1	3	5469.2984	0.0017	0.020
3	1	3	2	1	2	5949.2717	-0.0080	0.020
3	0	3	2	0	2	6164.8250	-0.0056	0.020
3	2	2	2	2	1	6187.9039	0.0228	0.020
3	2	1	2	2	0	6211.0662	-0.0172	0.020
3	1	2	2	1	1	6419.4560	0.0161	0.020
2	1	2	1	0	1	7058.8350	0.0034	0.020
4	1	4	3	1	3	7925.9038	0.0212	0.020
4	0	4	3	0	3	8193.0161	-0.0130	0.020

Table S15. Measured rotational transitions of thenyl alcohol (conformer GG, parent isotopologue), residuals according to fit of Table S6 and assumed experimental uncertainties (all values in MHz).

J'	K_{-1}'	K_{+1}'	J''	K_{-1}''	K_{+1}''	Frequency	Residuals	Uncertainty
3	1	3	3	0	3	2087.0945	-0.0125	0.020
3	1	2	3	1	3	2284.9587	0.0001	0.020
2	1	2	2	0	2	2540.7420	-0.0087	0.020
2	0	2	1	1	0	2856.3808	0.0059	0.020
1	1	1	1	0	1	2886.6231	-0.0080	0.020
1	0	1	0	0	0	3079.7555	0.0119	0.020
2	0	2	1	1	1	3237.5628	0.0169	0.020
1	1	0	1	0	1	3267.7931	-0.0090	0.020
2	1	1	2	0	2	3684.2520	-0.0091	0.020
4	1	3	4	1	4	3797.3672	0.0092	0.020
3	1	2	3	0	3	4372.0836	0.0180	0.020
4	1	3	3	2	2	4892.9298	-0.0310	0.020
4	1	3	4	0	4	5393.4596	-0.0118	0.020
3	0	3	2	1	1	5415.7027	0.0047	0.020
5	1	4	5	1	5	5660.7639	0.0014	0.020
2	1	2	1	1	1	5778.2964	-0.0001	0.020
1	1	1	0	0	0	5966.3703	-0.0044	0.020
2	0	2	1	0	1	6124.1897	0.0127	0.020
1	1	0	0	0	0	6347.5402	-0.0054	0.020
2	1	1	1	1	0	6540.6484	0.0123	0.020
5	2	4	5	1	4	6543.7586	-0.0061	0.020
3	0	3	2	1	2	6559.2125	0.0041	0.020
5	1	4	5	0	5	6799.4814	-0.0048	0.020
4	2	3	4	1	3	7398.3262	-0.0022	0.020
5	2	3	5	1	4	7683.7468	0.0097	0.020
6	2	4	6	1	5	7718.7814	-0.0072	0.020
6	1	5	6	1	6	7837.1127	0.0020	0.020
4	2	2	4	1	3	7909.0457	0.0023	0.020
7	2	5	7	1	6	8101.0042	0.0007	0.020
3	1	3	3	0	3	2087.0945	-0.0125	0.020
3	1	2	3	1	3	2284.9587	0.0001	0.020
2	1	2	2	0	2	2540.7420	-0.0087	0.020
2	0	2	1	1	0	2856.3808	0.0059	0.020
1	1	1	1	0	1	2886.6231	-0.0080	0.020
1	0	1	0	0	0	3079.7555	0.0119	0.020
2	0	2	1	1	1	3237.5628	0.0169	0.020
1	1	0	1	0	1	3267.7931	-0.0090	0.020
2	1	1	2	0	2	3684.2520	-0.0091	0.020
4	1	3	4	1	4	3797.3672	0.0092	0.020
3	1	2	3	0	3	4372.0836	0.0180	0.020
4	1	3	3	2	2	4892.9298	-0.0310	0.020
4	1	3	4	0	4	5393.4596	-0.0118	0.020

3	0	3	2	1	1	5415.7027	0.0047	0.020
5	1	4	5	1	5	5660.7639	0.0014	0.020
2	1	2	1	1	1	5778.2964	-0.0001	0.020
1	1	1	0	0	0	5966.3703	-0.0044	0.020
2	0	2	1	0	1	6124.1897	0.0127	0.020
1	1	0	0	0	0	6347.5402	-0.0054	0.020
2	1	1	1	1	0	6540.6484	0.0123	0.020
5	2	4	5	1	4	6543.7586	-0.0061	0.020
3	0	3	2	1	2	6559.2125	0.0041	0.020
5	1	4	5	0	5	6799.4814	-0.0048	0.020
4	2	3	4	1	3	7398.3262	-0.0022	0.020
5	2	3	5	1	4	7683.7468	0.0097	0.020
6	2	4	6	1	5	7718.7814	-0.0072	0.020
6	1	5	6	1	6	7837.1127	0.0020	0.020
4	2	2	4	1	3	7909.0457	0.0023	0.020
7	2	5	7	1	6	8101.0042	0.0007	0.020

Table S16. Measured rotational transitions of thenyl alcohol (conformer GG, ^{34}S(1) isotopologue), and residuals according to fit of Table S6 and assumed experimental uncertainties (all values in MHz).

J'	K_{-1}'	K_{+1}'	J''	K_{-1}''	K_{+1}''	Frequency	Residuals	Uncertainty
1	1	1	1	0	1	2784.4841	-0.0080	0.020
1	0	1	0	0	0	3066.2983	-0.0007	0.020
1	1	0	1	0	1	3173.4597	-0.0183	0.020
2	0	2	1	1	1	3310.1372	0.0047	0.020
2	1	1	2	0	2	3600.4107	-0.0045	0.020
3	1	2	3	0	3	4308.4014	0.0023	0.020
4	1	3	4	0	4	5362.7453	-0.0026	0.020
2	1	2	1	1	1	5743.5885	-0.0040	0.020
1	1	1	0	0	0	5850.7861	-0.0050	0.020
2	0	2	1	0	1	6094.6129	-0.0116	0.020
1	1	0	0	0	0	6239.7738	-0.0032	0.020
2	1	1	1	1	0	6521.5639	0.0020	0.020
3	0	3	2	1	2	6615.8973	0.0089	0.020
5	1	4	5	0	5	6813.7494	0.0023	0.020
5	2	3	5	1	4	7421.5737	0.0173	0.020
6	2	4	6	1	5	7505.4270	-0.0013	0.020
4	2	2	4	1	3	7617.6589	-0.0174	0.020
3	2	1	3	1	2	7982.3946	0.0196	0.020

Table S17. Measured rotational transitions of thenyl alcohol (conformer GG, ^{13}C(2) isotopologue), residuals according to fit of Table S6 and assumed experimental uncertainties (all values in MHz).

J'	K_{-1}'	K_{+1}'	J''	K_{-1}''	K_{+1}''	Frequency	Residuals	Uncertainty
1	0	1	0	0	0	3042.1190	0.0027	0.020
1	1	0	1	0	1	3275.2115	-0.0077	0.020
2	1	1	2	0	2	3681.2748	-0.0101	0.020
3	1	2	3	0	3	4350.5640	0.0014	0.020
4	1	3	4	0	4	5343.0073	0.0270	0.020
2	1	2	1	1	1	5711.7245	0.0025	0.020
1	1	1	0	0	0	5944.8412	-0.0033	0.020
2	0	2	1	0	1	6050.6471	0.0116	0.020
3	0	3	2	1	2	6429.9171	-0.0072	0.020
2	1	1	1	1	0	6456.6983	-0.0029	0.020
5	1	4	5	0	5	6709.0327	-0.0142	0.020

Table S18. Measured rotational transitions of thenyl alcohol (conformer GG, ^{13}C(3) isotopologue), residuals according to fit of Table S6 and assumed experimental uncertainties (all values in MHz).

J´	K_{-1}´	K_{+1}´	*J*´´	K_{-1}´´	K_{+1}´´	Frequency	Residuals	Uncertainty
1	0	1	0	0	0	3043.1113	-0.0016	0.020
2	0	2	1	1	1	3185.6099	0.0037	0.020
1	1	0	1	0	1	3242.2462	0.0040	0.020
2	1	1	2	0	2	3653.1865	-0.0050	0.020
3	1	2	3	0	3	4331.6127	-0.0088	0.020
4	1	3	4	0	4	5338.8201	0.0086	0.020
2	1	2	1	1	1	5709.9213	0.0120	0.020
1	1	1	0	0	0	5909.0562	-0.0019	0.020
2	0	2	1	0	1	6051.5547	0.0033	0.020
2	1	1	1	1	0	6462.4951	-0.0056	0.020
3	0	3	2	1	2	6468.2434	-0.0078	0.020

Table S19. Measured rotational transitions of thenyl alcohol (conformer GG, ^{13}C(4) isotopologue), residuals according to fit of Table S6 and assumed experimental uncertainties (all values in MHz).

J'	K_{-1}'	K_{+1}'	J''	K_{-1}''	K_{+1}''	Frequency	Residuals	Uncertainty
1	0	1	0	0	0	3069.9168	0.0123	0.020
1	1	0	1	0	1	3192.9677	0.0019	0.020
2	1	1	2	0	2	3618.1156	-0.0037	0.020
3	1	2	3	0	3	4322.5726	-0.0218	0.020
4	1	3	4	0	4	5371.1802	0.0156	0.020
2	1	2	1	1	1	5752.0961	0.0099	0.020
1	1	1	0	0	0	5875.1712	0.0041	0.020
2	0	2	1	0	1	6102.3338	-0.0024	0.020
2	1	1	1	1	0	6527.4817	-0.0081	0.020
3	0	3	2	1	2	6607.0751	-0.0050	0.020

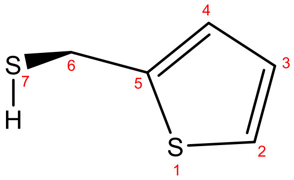
Table S20. Measured rotational transitions of thenyl alcohol (conformer GG, ^{13}C(5) isotopologue), residuals according to fit of Table S6 and assumed experimental uncertainties (all values in MHz).

J'	K_{-1}'	K_{+1}'	J''	K_{-1}''	K_{+1}''	Frequency	Residuals	Uncertainty
1	0	1	0	0	0	3078.0371	0.0008	0.020
1	1	0	1	0	1	3260.5199	0.0044	0.020
2	1	1	2	0	2	3676.9787	-0.0085	0.020
3	1	2	3	0	3	4364.9531	0.0247	0.020
4	1	3	4	0	4	5386.6584	-0.0022	0.020
2	1	2	1	1	1	5774.9442	0.0030	0.020
1	1	1	0	0	0	5957.4270	-0.0129	0.020
2	0	2	1	0	1	6120.6922	0.0019	0.020
2	1	1	1	1	0	6537.1631	0.0010	0.020
3	0	3	2	1	2	6560.9068	0.0000	0.020
5	1	4	5	0	5	6793.1159	-0.0060	0.020

Table S21. Measured rotational transitions of thenyl alcohol (conformer GG, ^{13}C(6) isotopologue), residuals according to fit of Table S6 and assumed experimental uncertainties (all values in MHz).

J'	K_{-1}'	K_{+1}'	J''	K_{-1}''	K_{+1}''	Frequency	Residuals	Uncertainty
1	0	1	0	0	0	3046.9234	0.0027	0.020
1	1	0	1	0	1	3261.6696	-0.0077	0.020
2	1	1	2	0	2	3668.5800	-0.0101	0.020
3	1	2	3	0	3	4339.5635	0.0014	0.020
4	1	3	4	0	4	5334.8507	0.0270	0.020
2	1	2	1	1	1	5720.7524	0.0025	0.020
1	1	1	0	0	0	5935.5228	-0.0033	0.020
2	0	2	1	0	1	6060.0139	0.0116	0.020
3	0	3	2	1	2	6457.8359	-0.0072	0.020
2	1	1	1	1	0	6466.9364	-0.0142	0.020

Table S22. Results of the effective structure (r_0) determination for the thenyl mercaptan conformer GG. The fitted parameters are compared with the theoretical predictions (theory, B3LYP-D3(BJ)/def2TZVP).

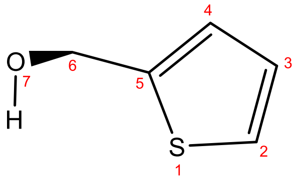


Fitted Parameters[a]	r_0	theory
α($S_{(1)}$-$C_{(2)}$-$C_{(3)}$) / deg	111.73(15)	111.66
α($C_{(2)}$-$C_{(3)}$-$C_{(4)}$) / deg	112.03(27)	112.41
α($C_{(3)}$-$C_{(4)}$-$C_{(5)}$) / deg	114.21(66)	113.30
α($C_{(4)}$-$C_{(5)}$-$C_{(6)}$) / deg	128.80(127)	127.08
α($C_{(5)}$-$C_{(6)}$-$S_{(7)}$) / deg	113.60(60)	114.73
τ($S_{(1)}$-$C_{(2)}$-$C_{(3)}$-$C_{(4)}$) / deg	-0.27(60)	-0.26
τ ($C_{(4)}$-$C_{(5)}$-$C_{(6)}$-$S_{(7)}$) / deg	-118.87(70)	-112.38
τ ($C_{(3)}$-$C_{(4)}$-$C_{(5)}$-$C_{(6)}$) / deg	183.58(202)	179.76
r ($C_{(2)}$-$S_{(1)}$) / Å	1.839(7)	1.842
r ($C_{(6)}$-$S_{(7)}$) / Å	1.708(4)	1.719
r ($C_{(5)}$-$C_{(6)}$) / Å	1.461(17)	1.487
r ($C_{(4)}$-$C_{(5)}$) / Å	1.383(5)	1.368

Table S23. Differences with the experimental rotational constants for the fitted structure of the thenyl mercaptan conformer GG of Table S22.

Isotopic species	Axis	Experiment / MHz	Exp.-Calc. / MHz
Parent	*A*	4209.193200	0.02
	B	1142.269010	0.02
	C	976.512730	0.01
^{34}S(7)	*A*	4199.998400	0.23
	B	1109.724900	0.03
	C	952.958600	0.01
^{34}S(1)	*A*	4121.710600	0.13
	B	1138.646300	0.04
	C	969.325200	0.00
^{13}C(6)	*A*	4175.794000	0.19
	B	1136.451900	0.01
	C	972.631500	0.01
^{13}C(5)	*A*	4198.731800	0.11
	B	1142.006800	0.02
	C	976.210300	0.08
^{13}C(4)	*A*	4140.402600	0.02
	B	1139.686800	0.02
	C	970.875700	0.00
^{13}C(3)	*A*	4177.154000	0.20
	B	1128.618000	0.01
	C	965.279800	0.03
^{13}C(2)	*A*	4198.989800	0.00
	B	1128.221300	0.02
	C	965.998400	0.02
RMS residuals			0.09

Table S24. Results of the effective structure determination for the thenyl alcohol conformer GG. The fitted parameters (r_0) are compared with the theoretical predictions (theory, B3LYP- GD3BJ /def2TZVP).



Fitted Parameters[a]	r_0	theory
α($S_{(1)}$-$C_{(2)}$-$C_{(3)}$) / deg	111.61(17)	111.74
α($C_{(2)}$-$C_{(3)}$-$C_{(4)}$) / deg	112.26(19)	112.34
α($C_{(3)}$-$C_{(4)}$-$C_{(5)}$) / deg	112.78(40)	113.34
α($C_{(4)}$-$C_{(5)}$-$C_{(6)}$) / deg	127.19(65)	127.71
τ ($S_{(1)}$-$C_{(2)}$-$C_{(3)}$-$C_{(4)}$) / deg	-0.85(27)	0.06
τ ($C_{(2)}$-$S_{(1)}$-$C_{(5)}$-$C_{(6)}$) / deg	179.24(40)	179.53
r ($S_{(1)}$-$C_{(2)}$) / Å	1.715(3)	1.718
r ($C_{(4)}$-$C_{(5)}$) / Å	1.379(3)	1.368
r ($C_{(5)}$-$C_{(6)}$) / Å	1.499(8)	1.494

Table S25. Differences with the experimental rotational constants for the fitted structure of the thenyl alcohol conformer GG of Table S24.

Isotopic species	Axis	Experiment / MHz	Exp.-Calc. / MHz
Parent	*A*	4617.10	0.13
	B	1730.46	0.02
	C	1349.29	0.03
^{34}S(1)	*A*	4512.15	0.02
	B	1727.64	0.03
	C	1338.66	0.05
^{13}C(6)	*A*	4598.61	0.06
	B	1710.01	0.01
	C	1336.92	0.03
^{13}C(5)	*A*	4608.99	0.02
	B	1729.57	0.07
	C	1348.46	0.06
^{13}C(4)	*A*	4534.08	0.15
	B	1728.80	0.06
	C	1341.10	0.03
^{13}C(3)	*A*	4575.66	0.02
	B	1709.71	0.01
	C	1333.41	0.02
^{13}C(2)	*A*	4610.04	0.03
	B	1707.30	0.02
	C	1334.81	0.03
RMS residuals			0.05

Table S26. Substitution coordinates for conformer GG of thenyl mercaptan (theoretical predictions in Table S1).

	Furfuryl mercaptan - GG´		
	a / Å[a]	*b* / Å	*c* / Å
C(2)[b]	2.333(2)[c]	0.461(10)	0.292(15)
C(3)	2.288(2)	0.901(6)	0.358(15)
C(4)	1.002(3)	1.419(2)	[0.000]
C(5)	[0.000][d]	0.42(3)	0.35(3)
C(6)	1.299(3)	0.617(6)	0.767(5)
S(1)	0.825(3)	1.127(2)	1.18(2)
S(7)	2.5462(11)	0.145(19)	0.342(8)

[a] Principal inertial axes labeled *a*, *b*, *c* (coordinate signs from the calculation in Table S1). [b] Notation according to Scheme of Table S1. [c] Uncertainties calculated according to Costain's rule: δz=0.0015/z (Å).

Table S27. Substitution coordinates for conformer GG of thenyl alcohol (theoretical predictions in Table S2).

	Furfuryl mercaptan - GG´		
	a / Å[a]	*b* / Å	*c* / Å
C(2)[b]	1.987(2)[c]	0.372(10)	0.18(2)
C(3)	1.873(2)	0.988(3)	0.20(2)
C(4)	0.529(8)	1.421(3)	[0.000][d]
C(5)	0.31(2)	0.370(16)	0.24(2)
C(6)	1.808(2)	0.459(8)	0.488(7)
S(1)	0.477(6)	1.135(2)	0.11(2)

[a] Principal inertial axes labeled *a*, *b*, *c* (coordinate signs from the calculation in Table S1). [b] Notation according to Scheme of Table S2. [c] Uncertainties calculated according to Costain's rule: $\delta z=0.0015/z$ (Å).

Table S28. Analysis of the rotational spectrum of ^{34}S-thenyl alcohol···$H_2{}^{16}O$.

	^{34}S-TA···$H_2{}^{16}O$
	0^-
A / MHz[a]	2168.300(20)
B / MHz	1257.7403(97)
C / MHz	1096.2325(53)
D_J / kHz	[0.7557][d]
D_{JK} / kHz	[1.987]
D_K / kHz	[-0.71]
d_1 / Hz	[0.0525]
d_2 / Hz	[-0.0414]
N[b]	5
σ / kHz	8.3

[a]Rotational constants (A, B, C), Watson's S-reduction centrifugal distortion constants (D_J, D_{JK}, D_K, d_1, d_2). [b]Number of transitions (N) and rms deviation (σ) of the fit. [c]Standard errors in parentheses in units of the last digit. [d]Values in square brackets were kept fixed in the fit.

Table S29. Analysis of the rotational spectrum of thenyl alcohol···$H_2{}^{18}O$.

	TA···$H_2{}^{18}O$	
	0^-	0^+
A / MHz[a]	2116.6372(32)[c]	2116.6784(80)
B / MHz	1244.0252(43)	1244.0195(69)
C / MHz	1070.7447(30)	1070.7979(48)
D_J / kHz	[0.7557][d]	
D_{JK} / kHz	[1.987]	
D_K / kHz	[-0.72]	
d_1 / Hz	[0.0525]	
d_2 / Hz	[-0.0414]	
N[b]	20	
σ / kHz	19.0	

[a]Rotational constants (A, B, C), Watson's S-reduction centrifugal distortion constants (D_J, D_{JK}, D_K, d_1, d_2). [b]Number of transitions (N) and rms deviation (σ) of the fit. [c]Standard errors in parentheses in units of the last digit. [d]Values in square brackets were kept fixed in the fit.

Table S30. Measured rotational transitions for isomer I of thenyl alcohol···$H_2{}^{16}O$, residuals according to fit of Table 3 and assumed experimental uncertainties (all values in MHz).

J'	K_{-1}'	K_{+1}'	v'	J''	K_{-1}''	K_{+1}''	v''	Frequency[1]	Residuals	Uncertainty
1	0	1	0	0	0	0	0	2369.1145	0.0016	0.020
5	2	3	0	5	1	4	0	2512.4843	0.0112	0.020
4	2	2	0	4	1	3	0	2534.1586	0.0048	0.020
3	2	1	0	3	1	2	0	2650.3479	-0.0178	0.020
3	2	1	1	3	1	2	1	2650.5536	-0.0181	0.020
5	1	4	0	5	0	5	0	2676.1368	-0.0334	0.020
2	2	0	0	2	1	1	0	2804.9603	-0.0105	0.020
2	2	0	1	2	1	1	1	2805.1660	0.0063	0.020
2	2	1	0	2	1	2	0	3273.6624	0.0078	0.020
1	1	1	0	0	0	0	0	3297.5756	-0.0101	0.020
1	1	1	1	0	0	0	1	3297.7087	0.0019	0.020
3	2	2	0	3	1	3	0	3529.3369	0.0001	0.020
2	0	2	0	1	1	1	0	3790.1425	-0.0143	0.020
4	2	3	1	4	1	4	1	3874.4798	-0.0111	0.020
4	2	3	0	4	1	4	0	3874.6250	-0.0048	0.020
5	2	4	0	5	1	5	0	4309.6479	-0.0132	0.020
3	1	2	0	2	2	1	0	4552.9422	0.0130	0.020
2	1	2	0	1	1	1	0	4575.4515	0.0053	0.020
2	1	2	1	1	1	1	1	4575.5968	-0.0065	0.020
5	3	2	0	5	2	3	0	4644.4317	0.0185	0.020
2	0	2	0	1	0	1	0	4718.6278	-0.0018	0.020
2	0	2	1	1	0	1	1	4718.7609	0.0108	0.020
4	3	1	0	4	2	2	0	4844.5468	0.0096	0.020
2	1	1	0	1	1	0	0	4900.9533	-0.0001	0.020
3	3	0	0	3	2	1	0	4966.1456	0.0105	0.020
3	3	0	1	3	2	1	1	4966.4360	0.0367	0.020
3	3	1	0	3	2	2	0	5060.7331	0.0107	0.020
4	3	2	0	4	2	3	0	5111.0161	0.0036	0.020
5	3	3	0	5	2	4	0	5207.5036	0.0039	0.020
2	1	2	0	1	0	1	0	5503.9126	-0.0064	0.020
2	1	2	1	1	0	1	1	5504.1426	-0.0007	0.020
3	0	3	0	2	1	2	0	6245.4738	0.0006	0.020
3	0	3	1	2	1	2	1	6245.6069	0.0279	0.020
3	1	3	0	2	1	2	0	6851.5312	-0.0099	0.020
3	1	3	1	2	1	2	1	6851.7732	-0.0109	0.020
3	0	3	0	2	0	2	0	7030.7586	-0.0039	0.020
3	0	3	1	2	0	2	1	7030.9644	-0.0079	0.020
3	2	2	0	2	2	1	0	7107.2298	0.0065	0.020
3	2	2	1	2	2	1	1	7107.3750	-0.0098	0.020
3	2	1	0	2	2	0	0	7183.7252	0.0062	0.020
3	2	1	1	2	2	0	1	7183.8341	0.0019	0.020
3	1	3	1	2	0	2	1	7637.1791	0.0016	0.020
3	1	2	0	2	1	1	0	7338.3255	0.0014	0.020

3	1	3	0	2	0	2	0	7636.8282	-0.0023	0.020
2	2	1	0	1	1	0	0	7686.3245	-0.0238	0.020
2	2	1	1	1	1	0	1	7686.5907	-0.0173	0.020
2	2	0	0	1	1	1	0	7868.6742	-0.0025	0.020
2	2	0	1	1	1	1	1	7868.8678	-0.0064	0.020
4	0	4	0	3	0	3	0	9295.4477	-0.0007	0.005
4	0	4	1	3	0	3	1	9295.7718	0.0001	0.005
4	1	3	0	3	1	2	0	9757.8591	0.0033	0.005
4	1	3	1	3	1	2	1	9758.0039	0.0015	0.005
5	1	5	0	4	1	4	0	11366.6547	-0.0002	0.005
5	1	5	1	4	1	4	1	11367.0909	0.0010	0.005
5	0	5	0	4	0	4	0	11517.5665	-0.0014	0.005
5	0	5	1	4	0	4	1	11518.0158	-0.0001	0.005
5	1	4	0	4	1	3	0	12150.2222	0.0020	0.005
5	1	4	1	4	1	3	1	12150.4389	0.0017	0.005
6	0	6	0	5	1	5	0	13439.2818	0.0036	0.005
6	0	6	1	5	1	5	1	13439.7116	0.0021	0.005
6	1	6	0	5	1	5	0	13605.1982	0.0004	0.005
6	1	6	1	5	1	5	1	13605.7372	0.0005	0.005
6	0	6	0	5	0	5	0	13714.6254	-0.0012	0.005
6	0	6	1	5	0	5	1	13715.1925	-0.0019	0.005
6	1	6	0	5	0	5	0	13880.5417	-0.0045	0.005
6	1	6	1	5	0	5	1	13881.2196	-0.0021	0.005
6	3	3	0	5	3	2	0	14362.6386	-0.0013	0.005
6	3	3	1	5	3	2	1	14362.8508	-0.0035	0.005
6	1	5	0	5	1	4	0	14504.1988	0.0004	0.005
6	1	5	1	5	1	4	1	14504.5141	0.0003	0.005
7	1	7	0	6	1	6	0	15833.1422	0.0009	0.005
7	1	7	1	6	1	6	1	15833.7882	0.0012	0.005

Table S31. Measured rotational transitions for isomer I of ^{34}S-thenyl alcohol···$H_2{}^{16}O$, residuals according to fit of Table S28 and assumed experimental uncertainties (all values in MHz).

J´	*K*$_{-1}$´	*K*$_{+1}$´	*v*´	*J*´´	*K*$_{-1}$´´	*K*$_{+1}$´´	*v*´´	Frequency	Residuals	Uncertainty
2	0	2	0	1	0	1	0	4688.2874	0.0041	0.020
2	1	2	0	1	0	1	0	5456.9518	-0.0086	0.020
3	0	3	0	2	1	2	0	6216.4500	-0.0084	0.020
3	1	3	0	2	1	2	0	6807.9468	-0.0019	0.020
3	0	3	0	2	0	2	0	6985.1489	0.0133	0.020

Table S32. Measured rotational transitions for isomer I of thenyl alcohol···$H_2^{18}O$, residuals according to fit of Table S29 and assumed experimental uncertainties (all values in MHz).

J'	K_{-1}'	K_{+1}'	v'	J''	K_{-1}''	K_{+1}''	v''	Frequency	Residuals	Uncertainty
2	1	2	0	1	1	1	0	4456.2375	0.0128	0.020
2	1	2	1	1	1	1	1	4456.3750	-0.0047	0.020
4	3	1	0	4	2	2	0	4557.6000	-0.0007	0.020
4	3	1	1	4	2	2	1	4557.8375	0.0014	0.020
2	0	2	0	1	0	1	0	4606.1750	-0.0060	0.020
2	0	2	1	1	0	1	1	4606.2875	-0.0052	0.020
3	3	0	0	3	2	1	0	4697.8875	-0.0093	0.020
2	1	1	0	1	1	0	0	4802.7875	-0.0044	0.020
2	1	1	1	1	1	0	1	4802.8000	-0.0274	0.020
3	3	1	0	3	2	2	0	4809.8625	-0.0406	0.020
4	3	2	0	4	2	3	0	4869.4000	0.0468	0.020
2	1	2	0	1	0	1	0	5328.8500	0.0094	0.020
3	0	3	0	2	1	2	0	6130.8875	-0.0156	0.020
3	0	3	1	2	1	2	1	6131.0250	0.0073	0.020
3	1	3	0	2	1	2	0	6670.5750	0.0064	0.020
3	1	3	1	2	1	2	1	6670.8000	-0.0107	0.020
3	0	3	0	2	0	2	0	6853.5625	-0.0002	0.020
3	0	3	1	2	0	2	1	6853.7625	-0.0052	0.020
3	2	2	0	2	2	1	0	6944.1875	0.0015	0.020
3	2	2	1	2	2	1	1	6944.3625	0.0335	0.020

Table S33. Analysis of the rotational spectrum of thenyl mercaptan···$H_2^{18}O$.

	TM···$H_2^{18}O$	
	0^-	0^+
A / MHz[a]	1767.39(15)[c]	1767.95(15)
B / MHz	981.9457(35)	981.8828(35)
C / MHz	825.7900(35)	825.9427(35)
D_J / kHz	[0.2403][d]	
D_{JK} / kHz	[3.122]	
D_K / kHz	[0.]	
d_1 / Hz	[0.0228]	
d_2 / Hz	[0.]	
N[b]	16	
σ / kHz	13.9	

[a]Rotational constants (A, B, C), Watson's S-reduction centrifugal distortion constants (D_J, D_{JK}, D_K, d_1, d_2). [b]Number of transitions (N) and rms deviation (σ) of the fit. [c]Standard errors in parentheses in units of the last digit. [d]Values in square brackets were kept fixed in the fit.

Table S34. Measured rotational transitions for isomer I of thenyl mercaptan···$H_2{}^{16}O$, residuals according to fit of Table 4 and assumed experimental uncertainties (all values in MHz).

J'	K_{-1}'	K_{+1}'	v'	J''	K_{-1}''	K_{+1}''	v''	Frequency[1]	Residuals	Uncertainty
2	1	2	0	1	1	1	0	3520.5126	-0.0084	0.020
2	1	2	1	1	1	1	1	3520.9298	0.0000	0.020
2	0	2	0	1	0	1	0	3642.9644	-0.0068	0.020
2	0	2	1	1	0	1	1	3643.1909	-0.0063	0.020
2	1	1	0	1	1	0	0	3795.1112	-0.0155	0.020
3	1	3	0	2	1	2	0	5271.9355	0.0066	0.020
3	1	3	1	2	1	2	1	5272.5792	-0.0006	0.020
3	0	3	0	2	0	2	0	5428.3977	-0.0024	0.020
3	0	3	1	2	0	2	1	5428.8983	0.0069	0.020
3	2	2	0	2	2	1	0	5486.6672	0.0020	0.020
3	2	2	1	2	2	1	1	5486.9056	-0.0010	0.020
3	2	1	0	2	2	0	0	5544.9963	-0.0089	0.020
3	1	2	0	2	1	1	0	5682.8022	-0.0249	0.020
4	1	4	0	3	1	3	0	7014.0600	-0.0004	0.020
4	1	4	1	3	1	3	1	7014.9899	0.0004	0.020
4	0	4	0	3	0	3	0	7176.3873	-0.0061	0.020
4	0	4	1	3	0	3	1	7177.2814	0.0000	0.020
4	2	3	0	3	2	2	0	7303.9413	0.0106	0.020
4	2	3	1	3	2	2	0	7304.2989	-0.0045	0.020
4	3	2	0	3	3	1	0	7342.3147	-0.0181	0.020
4	3	2	1	3	3	1	1	7342.5412	-0.0023	0.020
4	3	1	0	3	3	0	0	7348.3586	-0.0060	0.020
4	3	1	1	3	3	0	1	7348.5374	0.0040	0.020
4	2	2	0	3	2	1	0	7443.1062	-0.0003	0.020
4	2	2	1	3	2	1	1	7442.9154	0.0015	0.020
4	1	3	0	3	1	2	0	7557.2371	-0.0118	0.020
6	1	6	0	5	1	5	0	10467.5017	-0.0007	0.005
6	0	6	0	5	0	5	0	10576.4659	0.0011	0.005
6	3	4	0	5	3	3	0	11029.4824	-0.0025	0.005
6	3	3	0	5	3	2	0	11083.1611	0.0034	0.005
6	1	5	0	5	1	4	0	11237.6568	0.0040	0.005
7	1	7	0	6	1	6	0	12180.2197	-0.0007	0.005
7	0	7	0	6	0	6	0	12254.8698	-0.0002	0.005
7	5	3	0	6	5	2	0	12854.0600	0.0092	0.005
7	5	2	0	6	5	1	0	12854.2034	-0.0063	0.005
7	4	4	0	6	4	3	0	12872.9374	-0.0043	0.005
7	1	6	0	6	1	5	0	13026.8066	0.0023	0.005
8	1	8	0	7	1	7	0	13885.7804	0.0009	0.005
8	0	8	0	7	0	7	0	13933.0098	0.0007	0.005
8	1	7	0	7	1	6	0	14773.6320	-0.0032	0.005
9	0	9	0	8	0	8	0	15614.3100	-0.0001	0.005

Table S35. Measured rotational transitions for isomer I of thenyl mercaptan···$H_2{}^{18}O$, residuals according to fit of Table S31 and assumed experimental uncertainties (all values in MHz).

J'	K_{-1}'	K_{+1}'	J''	K_{-1}''	K_{+1}''	Frequency	Residuals	Uncertainty
2	1	1	1	1	1	3459.6875	-0.0024	0.020
2	0	0	1	0	1	3594.6625	0.0001	0.020
2	1	1	1	1	0	3771.6000	0.0284	0.020
3	1	1	2	1	2	5177.2041	0.0210	0.020
3	0	0	2	0	2	5341.9250	-0.0021	0.020
3	2	2	2	2	1	5423.3375	-0.0380	0.020
3	2	2	2	2	0	5504.9000	0.0011	0.020
3	1	1	2	1	1	5643.2250	0.0005	0.020

Table S36. B2PLYP-D3(BJ) and ωB97XD DFT predictions for the thenyl alcohol monohydrate TA···H_2O.

	Isomer 1^{c}	**Isomer 2**
	GG-Wa	**AG´-Wa**
A / MHz^{a}	2230.47/2235.29	2327.08/2349.85
B / MHz	1277.92/1271.40	1175.58/1165.89
C / MHz	1100.07/1113.63	1061.19/1034.87
D_J / kHz	0.5823/0.6003	0.6160/0.5691
D_{JK} / kHz	1.7759/1.6918	1.2166/1.0798
D_K / kHz	-0.7943/-0.8142	0.1492/0.4294
d_1 / kHz	0.0672/0.0587	0.0435/0.0453
d_2 / kHz	-0.0626/-0.0478	-0.0530/-0.0526
$\|\mu_a\|$ / D	2.44/2.54	1.68/1.45
$\|\mu_b\|$ / D	1.87/1.62	2.28/2.38
$\|\mu_c\|$ / D	0.33/0.15	0.19/0.11
ΔE /kJ mol$^{-1\ b}$	0.00/0.00	4.01/3.35
ΔG /kJ mol^{-1}	0.00/0.00	3.53/2.96

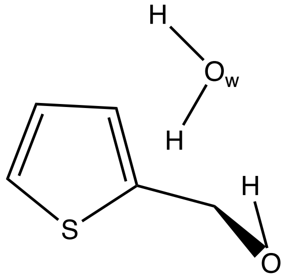
[a] Rotational constants (A, B, C), Watson's S-reduction centrifugal distortion constants (D_J, D_{JK}, D_K, d_1, d_2) and electric dipole moments (μ_α, α = a, b, c). [b] Relative energies corrected with the zero-point energy (ZPE), Gibbs energy (ΔG, 298K, 1 atm) and complexation energy (including BSSE corrections). [c] B2PLYP-D3(BJ) and ωB97XD values, respectively (basis set def2TZVP).

Table S37. Substitution coordinates for the oxygen atom and the ring sulfur in thenyl alcohol···H_2O using the Kraitchman equations (unsigned), and comparison with the DFT prediction (B3LYP- GD3BJ /def2TZVP).

	Thenyl Alcohol – water		
	a / Å[a]	*b* / Å	*c* / Å
O_w	1.73173(88)[b]	1.99122(76)	0.6887(22)
S_{ring}	0.82742(193)	0.87877(182)	0.8052(20)
	B3LYP- GD3BJ /def2TZVP		
O_w	-1.7053	-1.9710	-0.7531
S_{ring}	0.8616	0.9292	-0.7565

[a] Principal inertial axes denoted *a*, *b*, *c*. [a] Uncertainties according to Costain's estimation: $\delta z=0.0015/z$.

Table S38. Results of the effective structure (r_0) determination for thenyl alcohol···H_2O. The fitted parameters are compared with the theoretical predictions (theory, B3LYP-GD3BJ /def2TZVP). The residuals of the fit of the experimental rotational constants are shown below.



Fitted Parameters[a]	r_0	theory
r (H···O$_w$) / Å	1.984(4)	1.965
∠(O-H···O$_w$) / deg	160.773(65)	159.63
τ(C-O-H···O$_w$) / deg	-39.37(10)	-32.99

Isotopic species	Axis	Experiment / MHz	Exp.-Calc. / MHz
Parent	*A*	2194.41	0.23
	B	1265.93	0.01
	C	1103.18	0.03
^{34}S	*A*	2116.65	-1.04
	B	1244.03	-0.23
	C	1070.74	-0.47
^{18}O	*A*	2168.30	0.13
	B	1257.74	-0.34
	C	1096.23	-0.25
RMS residuals			0.40

Table S39. Equilibrium coordinates for thenyl alcohol···H_2O according to the DFT prediction (B3LYP- GD3BJ /def2TZVP).

Atom	*a* / Å[a]	*b* / Å	*c* / Å
C	2.1431	-0.1774	-0.4524
C	1.8920	-0.9513	0.6425
C	0.6390	-0.6443	1.2455
C	-0.0402	0.3591	0.6064
S	0.8616	0.9292	-0.7565
C	-1.3948	0.9129	0.9342
O	-2.3222	0.7897	-0.1288
H	3.0061	-0.1994	-1.0976
H	2.5687	-1.7110	1.0059
H	0.2515	-1.1420	2.1240
H	-1.3316	1.9801	1.1551
H	-1.7493	0.4096	1.8427
H	-2.3383	-0.1449	-0.3985
O_w	-1.7053	-1.9710	-0.7531
H	-0.8245	-1.8179	-0.3818
H	-1.5644	-2.1403	-1.6909

[a] Principal inertial axes labeled *a*, *b*, *c*.

Table S40. B2PLYP-D3(BJ) and ωB97XD DFT predictions for the thenyl mercaptan monohydrate TM···H_2O.

	Isomer 1[b]	**Isomer 2**
	GG-Wa	**GG´-Wdπ**
A / MHz[a]	1925.02/1937.70	1882.58/1883.47
B / MHz	981.27/979.56	990.28/990.14
C / MHz	861.37/865.32	845.09/841.60
D_J / kHz	0.2402/0.1766	0.1628/0.1429
D_{JK} / kHz	2.4644/1.8866	1.3652/1.4107
D_K / kHz	-0.721/-0.3641	0.1145/-0.0275
d_1 / kHz	0.0309/0.0077	0.0040/0.0019
d_2 / *k*Hz	0.0119/0.0154	0.0010/-0.0014
$\lvert\mu_a\rvert$ / D	2.62/2.54	1.20/1.39
$\lvert\mu_b\rvert$ / D	0.79/1.22	3.07/2.99
$\lvert\mu_c\rvert$ / D	0.40/0.72	1.04/1.04
ΔE/ kJ mol^{-1}	0.00/0.00	0.77/1.08
ΔG /kJ mol^{-1}	0.00/0.00	2.73/2.45

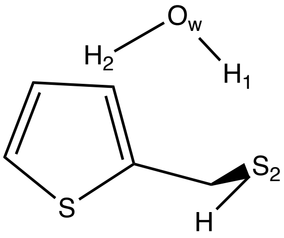
[a]Parameter definition as in Table 36. [b] B2PLYP-D3(BJ) and ωB97XD values, respectively (basis set def2TZVP).

Table S41. Substitution coordinates for the oxygen atom in thenyl mercaptan···H_2O using the Kraitchman equations (unsigned), and comparison with the DFT prediction (B3LYP- GD3BJ /def2TZVP).

	Thenyl Mercaptan – water		
	a / Å[a]	*b* / Å	*c* / Å
O_w	0.3709(57)[b]	2.67581(82)	0.4363(55)
	B3LYP- GD3BJ /def2TZVP		
O_w	0.3068	-2.6505	-0.4525

[a] Principal inertial axes denoted *a*, *b*, *c*. [a] Uncertainties according to Costain's estimation: $\delta z=0.0015/z$.

Table S42. Results of the effective structure determination for thenyl mercaptan···H_2O. The fitted parameters (r_0) are compared with the theoretical predictions (theory, B3LYP-GD3BJ /def2TZVP). The differences with the experimental rotational constants for the fitted structure are shown below.



Fitted Parameters[a]	r_0	theory
r (H_1···S(2)) / Å	2.634(18)	2.579
∠(C-S(2)···H_1) / deg	74.07(63)	79.88
τ(C-C-S(2)···H_1) / deg	95.09(21)	94.52

Isotopic species	Axis	Experiment / MHz	Exp.-Calc. / MHz
Parent	*A*	1861.92	-1.31
	B	983.11	-0.22
	C	845.81	0.05
^{18}O	*A*	1767.39	-2.17
	B	981.95	0.53
	C	825.79	-0.25
RMS residuals			1.05

Table S43. Equilibrium coordinates for thenyl mercaptan···H_2O according to the DFT prediction (B3LYP- GD3BJ /def2TZVP).

Atom	*a* / Å[a]	*b* / Å	*c* / Å
C	-2.3747	-0.0484	-0.3231
C	-2.1190	-0.4664	0.9519
C	-0.8409	-0.0522	1.4151
C	-0.1429	0.6753	0.4904
S	-1.0644	0.8614	-0.9614
C	1.2469	1.1916	0.5932
S	2.5311	0.0461	-0.0801
H	-3.2626	-0.2083	-0.9119
H	-2.8165	-1.0457	1.5391
H	-0.4414	-0.3012	2.3882
H	1.5215	1.3116	1.6405
H	1.3659	2.1579	0.1072
H	2.1367	0.1134	-1.3623
O_w	0.3068	-2.6505	-0.4525
H	0.9912	-2.0193	-0.1893
H	-0.5202	-2.2096	-0.2269

[a] Principal inertial axes labeled *a*, *b*, *c*.