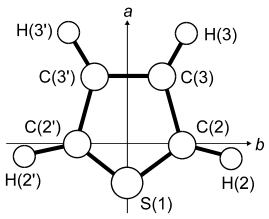
514 **C_4H_4S** **Thiophene** **C_{2v}**

ED, MW, vibrational spectroscopy, *ab initio* and DFT calculations

r_e [a])	Å [b])
C(2)–H	1.085(2)
C(3)–H	1.088 [c])
C(2)=C(3)	1.372(3)
S–C	1.704(2)
C(3)–C(3')	1.421(4)

θ_e [a])	deg [b])
H–C–S	119.9(3)
H–C(3)–C(3')	124.4(4)
C–S–C	92.4(2)
S–C–C	111.6 [d])
C–C=C	112.2 [d])
H–C(2)=C(3)	128.5 [d])
H–C(3)=C(2)	123.4 [d])

r_g	Å [c])
C(2)–H	1.104
C(3)–H	1.108
C(2)=C(3)	1.380
S–C	1.712
C(3)–C(3')	1.429



The electron diffraction intensities from [1] were reanalyzed.
The nozzle temperature was 300 K.

[a]) Potential function with quadratic and cubic force constants from B3LYP/6-311+G* calculations empirically improved by harmonic scale factors were used in the analysis of all the available experimental data.
[b]) Uncertainties were unidentified, probably estimated standard errors.
[c]) Uncertainties were not given in the original paper.
[d]) Dependent parameter.

Kochikov, I.V., Tarasov, Yu.I., Spiridonov, V.P., Kuramshina, G.M., Rankin, D.W.H., Saakjan, A.S., Yagola, A.G.: J. Mol. Struct. **567-568** (2001) 29.
[1] Liescheski, P.B., Rankin, D.W.H.: J. Mol. Struct. **178** (1988) 227.

II/25C (**3**, 1570)