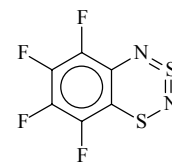


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 $C_6F_4N_2S_2$ 5,6,7,8-Tetrafluoro-1,3,4- δ^2 ,2,4-benzodithiadiazine C_s ED, *ab initio* and DFT calculations

r_{hl} ^{a)}	\AA ^{b)}	θ_{hl} ^{a)}	deg ^{b)}
C(4a)–C(8a)	1.405(8)	C(5)–C(4a)–C(8a)	116.2(5)
C(8a)–C(8)	1.370(8)	C(6)–C(5)–C(4a)	122.3(5)
C(8)–C(7)	1.397(6)	C(5)–C(6)–C(7)	119.1(6)
C(7)–C(6)	1.372(8)	F–C(5)–C(4a)	120.2(7)
C(6)–C(5)	1.395(6)	F–C(6)–C(5)	119.5(8)
C(5)–C(4a)	1.398(8)	F–C(7)–C(6)	120.9(8)
C(4a)–N(4)	1.396(7)	F–C(8)–C(7)	117.4(8)
C(8a)–S(1)	1.812(9)	N–C(4a)–C(8a)	125.4(7)
N(2)–S(1)	1.723(8)	S(1)–N(2)=S(3)	122.8(5)
S(3)=N(2)	1.553(3)	N(2)–S(1)–C(8a)	104.5(3)
N(4)=S(3)	1.552(3)	S(1)–C(8a)–C(4a)	124.6(6)
C–F ^{c)}	1.330(5)	N–C(4a)–C(8a)–S(1)	0.0 ^{d)}
		S(3)=N(2)–S(1)–C(8a)	0.0 ^{d)}
		N(2)–S(1)–C(8a)–C(4a)	0.0 ^{d)}
		S(1)–C(8a)–C(4a)–C(5)	180.0 ^{d)}



Differences between similar parameters were restrained to the values from quantum chemical calculations.

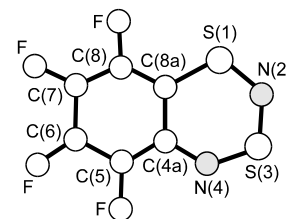
The nozzle temperature was 138...164 °C.

^{a)} Nonlinear kinematic effects were taken into account.

^{b)} Estimated standard errors.

^{c)} Average value.

^{d)} Assumed at the value from B3LYP/6-311+G* calculations.



Blockhuys, F., Hinchley, S.L., Marakov, A.Yu., Gatilov, Yu.V.,

Zibarev, A.V., Woollins, J.D., Rankin, D.W.H.: Chem. Eur. J. 7 (2001) 3592.