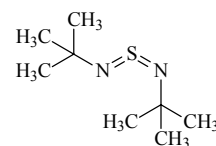


857 $\text{C}_8\text{H}_{18}\text{N}_2\text{S}$ *N,N'*-Bis(1,1-dimethylethyl)sulfur diimide C_s assumedED, *ab initio*
calculations

r_a	\AA^a	θ_a	deg^a
S=N(1)	1.538(3) ^{b)}	N=S=N	117.8(6)
S=N(2)	1.565(4) ^{b)}	C–C–H	109.6(4)
N(1)–C	1.462(4) ^{b)}	N(2)–C(1')–C(2')	115.6(6) ^{c)}
N(2)–C	1.470(4) ^{b)}	N(2)–C(1')–C(3',4')	105.4(5) ^{c)}
C(1')–C(2')	1.526(2) ^{b)}	N(1)–C(1)–C(3,4)	111.1(4) ^{c)}
C(1)–C(3)	1.526(2) ^{b)}	N(1)–C(1)–C(2)	103.8(6) ^{c)}
C–H	1.118(1)	C(3)–C(1)–C(2)	110.2(3)
		C(2')–C(1')–C(3')	110.0(3)
		S=N(1)–C(1)	125.9(6) ^{b)}
		S=N(2)–C(1')	116.7(7) ^{b)}
		tilt1(<i>t</i> -butyl) ^{d)}	–6.7(5)
		tilt1'(<i>t</i> -butyl) ^{d)}	–4.9(5)



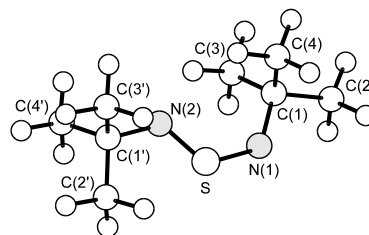
The methyl groups were assumed to have local C_{3v} symmetry and *t*-butyl groups local C_3 symmetry. MP2/cc-pVTZ calculations predicted the *E/Z* isomer (C–N=S=N fragments in *trans* and *cis* positions) to be more stable than the *E/E* isomer (both C–N=S=N fragments in *trans* positions) by 36.5 kJ mol^{–1}.

^{a)} Estimated standard errors.

^{b)} Differences between the C–C, C–N and S=N bond lengths and between the S=N–C bond angles were restrained to the values from MP2/cc-pVTZ" (*i.e.*, employing cc-pVTZ basis on S, N and the nearest-neighbor C atom, and cc-pVDZ on the methyl groups) calculations.

^{c)} Restrained to the value from MP2/cc-pVTZ" calculations.

^{d)} Tilt angles of the *t*-butyl groups with C(1) and C(1'), respectively, in the mirror plane of the molecule, a negative value when the *t*-butyl group tilts away from the S atom. Out-of-plane tilts are possible, but they were ignored.



Hinchley, S.E., Trickey, P., Robertson, H.E., Smart, B.A., Rankin, D.W.H., Leusser, D., Walfort, B., Stalke, D., Bühl, M., Obrey, S.J.: J. Chem. Soc., Dalton Trans. (2002) 4607.