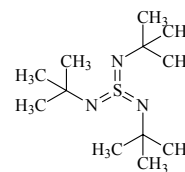


911 **C₁₂H₂₇N₃S**ED, *ab initio*
calculations***N,N',N''*-Tris(1,1-dimethylethyl)sulfur triimide** essentially **C_{3h}**

r_a	Å ^{a)}	θ_a	deg ^{a)}
S=N	1.535(3) ^{b)}	N–C–C ^{c)}	108.4(3)
N–C	1.473(5) ^{b)}	S=N–C	122.9(4)
C–C ^{c)}	1.508(2) ^{b)}	C–C–C ^{c)}	109.9(3) ^{b)}
C–H ^{c)}	1.129(3)	C–C–H	107.1(5) ^{d)}
		H–C–H ^{c)}	107.1(5)
		α (S=N) ^{e)}	173.0(5)
		twist(CH ₃)	53.4(23) ^{d)}
		twist(<i>t</i> -butyl) ^{f)}	188.5(7) ^{d)}

The ED analysis made assuming C₃ symmetry resulted in a slight twist of the *t*-butyl groups out of the plane, α (S=N) = 173.0(5)°. In contrast, MP2(fc)/6-31G* calculations predicted that S(NBu)₃ had C_{3h} symmetry, α (S=N) = 180°. This discrepancy can be ascribed to the shrinkage effect (apparent nonplanarity caused by vibration). The methyl groups were assumed to have local C_{3v} symmetry.

The nozzle temperature was 383 K.

^{a)} Estimated standard errors.

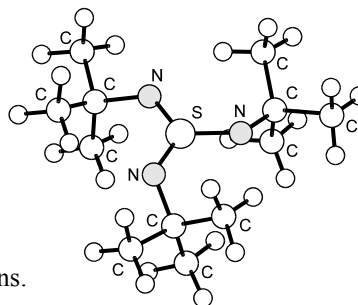
^{b)} Differences between the C–C, C–N and S=N bond lengths and between the C–C–C angles were restrained to the values from MP2/6-31G* calculations.

^{c)} Mean value.

^{d)} Restrained to the value from MP2/6-31G* calculations.

^{e)} Torsional angle N=S=N–C, α (S=N) = 180° when the S(NC)₃ core is planar.

^{f)} The *t*-butyl groups are effectively staggered with respect to the N=S bonds.



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