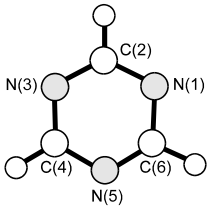
364 **$C_3H_3N_3$** **1,3,5-Triazine** **D_{3h}**

ED, IR, NMR,
ab initio calculations

r_α^0	Å [a])	θ_α^0	deg [a])
C–N	1.3368(1)	N–C–N [b])	126.18(9)
C–H	1.089(2)	C–N–C	113.82(9)

The equilibrium bond lengths r_e(C–N) and r_e(C–H) were estimated to be 1.329(2) Å and 1.077(3) Å, respectively, using the Morse constants determined from the data of MP2/6-31G* calculations.
The nozzle temperature was 387 K.



[a]) Estimated standard errors.
[b]) Dependent parameter.

Morrison, C.A., Smart, B.A., Rankin, D.W.H., Robertson, H.E., Pfeffer, M., Ruber, R., Bodenmüller, W., Macht, B., Ruoff, A., Typke, V.: J. Phys. Chem. A **101** (1997) 10029.

IR

r_0	Å [a])	θ_0	deg [a])
C–N	1.33679(4)	N–C–N	126.098(57)
C–H	1.0849(5)	C–N–C	113.900(57)

r_s	Å [a])	θ_s	deg [a])
C–N	1.33412(5)	N–C–N	126.037(7)
C–H	1.08682(7)	C–N–C	113.963(7)

The r_0 and r_s structures were derived from seven isotopomers.

[a]) Estimated standard errors.

Pfeffer, M., Martz, J., Steinmann, A., Ruoff, A., Typke, V.: J. Mol. Spectrosc. **200** (2000) 285.

Replaces II/25C (**3**, 1126)