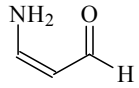
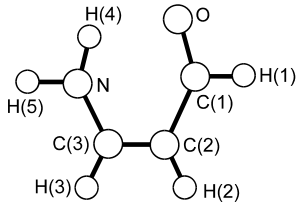
380 **C_3H_5NO** **(*Z*)-3-Amino-2-propenal** **C_s** assumed (*syn*)
ED, *ab initio* calculations
(*Z*)-3-Aminoacrylaldehyde
cis-3-Aminoacrolein



r_g	Å [a])
N–H [b])	1.002(26)
C–H [b])	1.086(20)
C(1)=O	1.232(7)
C(3)–N	1.358(26)
C(2)=C(3)	1.363(31)
C(1)–C(2)	1.424(18)

θ_α	deg [a])
H(4)–N–C	119.5(33)
H(5)–N–C	122.1(32)
H(2,3)–C=C	119.3(33)
H(1)–C–C	116.1(33)
O=C(1)–C(2)	127.0(32)
N–C(3)=C(2)	124.2(57)
C(1)–C(2)=C(3)	120.7(28)
C(2)=C(3)–N–H(5)	180.0 [c])
C(2)=C(3)–N–H(4)	0.0 [c])
C(1)–C(2)=C(3)–N	0.0 [c])
C(3)=C(2)–C(1)=O	0.0 [c])

Of the four possible forms of 3-aminoacrolein (*syn* and *anti* conformers of *cis* isomer and *syn* and *anti* conformers of *trans* isomer) the *syn* conformer (τ[O=C(1)–C(2)=C(3)] = 0°) of *cis* isomer was found to be the overwhelmingly dominant form (98(41) mol%) in agreement with the results of HF/6-31G* calculations. The presence of small amount of the *syn* conformer of *trans* isomer (2(41) mol%) was indicated. Structural differences between the *syn* conformers of *cis* and *trans* isomers were assumed at the values from *ab initio* calculations.
The temperature of the inlet tube was 135 °C.



[a]) Twice the estimated standard errors.
[b]) Average value.
[c]) Assumed.

Richardson, A.D., Hedberg, K., Wiberg, K.B., Rablen, P.R.: J. Mol. Struct. **445** (1998) 1.