245 **C_2H_3N** **Methyl isocyanide** **C_{3v}**
MW, *ab initio* calculations (MP2/cc-pCVQZ, CCSD(T)/cc-pCVQZ)
Isocyanomethane
$H_3C–N=C$

r_0	Å
N=C	1.1720(16)
C–N	1.4223(14)
C–H	1.0923(5)

θ_0	deg
H–C–N	109.35(3)

r_s [a])	Å
N=C	1.1699(21)
C–N	1.4209(16)
C–H	1.0937(17)

θ_s [a])	deg
H–C–N	109.37(8)

$r_m^{(1)}$ [b])	Å
N=C	1.1683(22)
C–N	1.4186(19)
C–H	1.0951(19)

$\theta_m^{(1)}$ [b])	deg
H–C–N	109.27(9)

$r_m^{(2)}$ [c])	Å
N=C	1.1708(13)
C–N	1.4181(8)
C–H	1.0988(8)

$\theta_m^{(2)}$ [c])	deg
H–C–N	108.91(12)

r_e [d])	Å
N=C	1.1666(6)
C–N	1.4259(3)
C–H	1.0902(20)

θ_e [d])	deg
H–C–N	109.47(15)

The best equilibrium structure, which was derived from high-level *ab initio* calculations, is r_e(C–H) = 1.086 Å, r_e(C–N) = 1.422 Å, r_e(N=C) = 1.169 Å, and θ_e(H–C–N) = 109.47°. The original paper also reports the results for which r(C–H) – r(C–D) was taken into account.

[a]) c_a = –0.008(14), $c_b = c_c$ = 0.115(72), in u^{½} Å, included in the fit.
[b]) c_a = –0.012(9), $c_b = c_c$ = 0.037(17), in u^{½} Å, included in the fit.
[c]) c_a = –0.177(20), $c_b = c_c$ = 0.008(17), in u^{½} Å, d_a = 0.179(21), $d_b = d_c$ = 0.120(78), in u^{½} Å^2, included in the fit.
[d]) Extrapolated from the r_z structure

Margulés, L., Demaison, J., Rudolph, H.D.: J. Mol. Struct. **599** (2001) 23.
Replaces II/25B(**3**, 690), MW (first part)