

1451 **C₃N****Cyanoethynyl****C_{∞v}**
C≡C–C≡NMW, *ab initio* calculations
(RCCSD(T))

	r_0 [Å]	r_s [Å]	r_e [Å] ^{a)}
C≡C	1.208(3)	1.206(3)	1.2116
C–C	1.378(3)	1.379(3)	1.3746
C≡N	1.158(3)	1.160(3)	1.1609

^{a)} r_e structure derived by converting the experimental rotational constants to equilibrium constants using vibration-rotation coupling constants derived from *ab initio* calculations.

McCarthy, M.C., Gottlieb, C.A., Thaddeus, P., Horn, M., Botschwina, P.: J. Chem. Phys. **103** (1995) 7820.