

Solvent Table

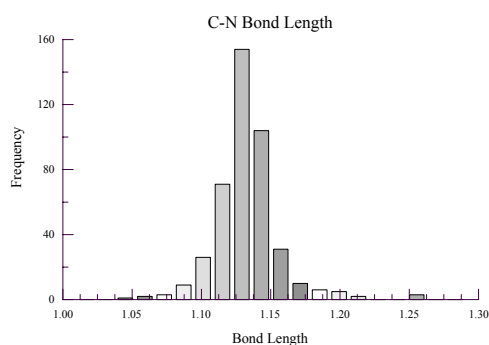
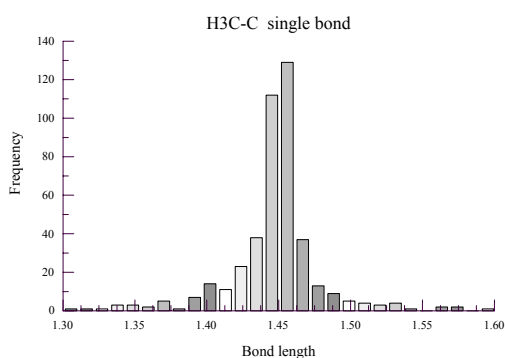
CH₃CN

Information

Formula C₂H₃N weight 41.05 amu

H₃C₁ - C₂ ≡ N₃

C1-C2 1.438 (64)
C2-N3 1.147 (76)
C1..N3 2.585 (ideal value for 180 angle)
C1..N3 2.581 (52)



Cambridge Crystallographic DataBase 5.24 April 2003.

Temperature < 90C, no disorder, no errors, R < 5%

Number of Bond Lengths 445

C1-C2

Minimum value: 1.064, Maximum value: 1.601, Median: 1.449, Arithmetic mean: 1.438,
Geometric mean: 1.436, Quadratic mean: 1.439, Harmonic mean: 1.434, Absolute mean:
1.438, Variance: 0.0041, Standard deviation: 0.064, Absolute deviation: 0.032, Standard error:
0.0030, Skewness: -3.557

C2-N3

Minimum value: 0.954, Maximum value: 1.655, Median: 1.133, Arithmetic mean: 1.147,
Geometric mean: 1.144, Quadratic mean: 1.149, Harmonic mean: 1.143, Absolute mean:
1.147, Variance: 0.0058, Standard deviation: 0.076, Absolute deviation: 0.034, Standard error:
0.0036, Skewness: 4.286

Orthogonal Coordinates

N3 1.4366 0.1173 0.1096
C2 0.2870 0.1266 -0.0726
C1 -1.1608 0.1383 -0.3021
H1 -1.6548 -0.6232 0.3422
H2 -1.5770 1.1416 -0.0590
H3 -1.3794 -0.0946 -1.3683