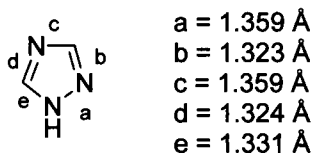
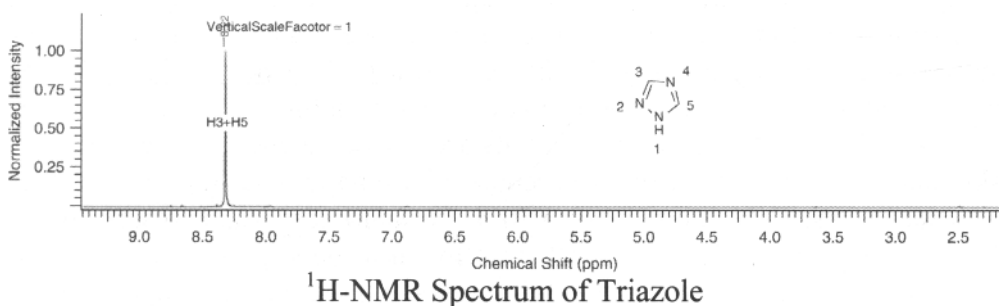


The bond lengths for the 1*H*-1,2,4-triazole are shown below,<sup>2</sup> which impact the coupling constants in their <sup>1</sup>H-NMR spectra.

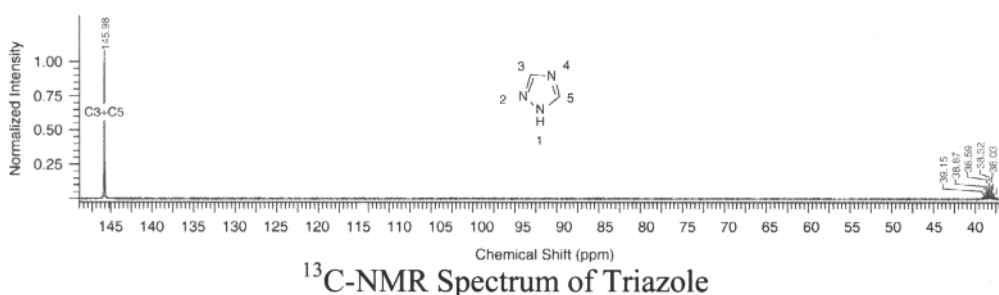


<sup>1</sup>H-1,2,4-Triazole's Bond Lengths

In 1,2,4-triazole's <sup>1</sup>H-NMR spectrum, the chemical shift for both H3 and H5 is the same (due to the tautomerization between the nitrogen atoms) at 8.32 ppm. Like other NH-containing heterocycles, the chemical shift of triazole's NH largely depends on the solvent used to do the NMR spectrum.



In 1,2,4-triazole's <sup>13</sup>C-NMR spectrum, the chemical shift for both C3 and C5 is the same again, due to the tautomerization between the nitrogen atoms, at 145.98 ppm.



In 1,2,3-triazole's <sup>1</sup>H-NMR spectrum, the chemical shift for both H4 and H5 is the same at 7.90 ppm. Like other NH-containing heterocycles, the chemical shift of triazole's NH largely depends on the solvent used to do the NMR spectrum. In 1,2,3-triazole's <sup>13</sup>C-NMR spectrum, the chemical shift for both C4 and C5 is the same at 130.9 ppm

In tetrazole's <sup>1</sup>H-NMR spectrum, the chemical shift for the H5 is at 9.50 ppm. Like other NH-containing heterocycles, the chemical shift of triazole's NH largely depends on the solvent used to do the NMR spectrum.