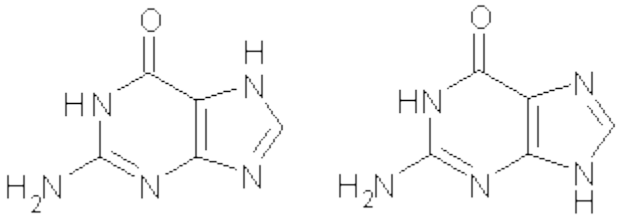
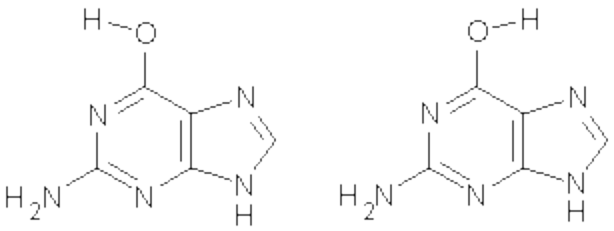
GAUNINE TAUTOMERS

Here's another fine paper from the Alonso group employing laser ablation molecular beam Fourier transform microwave spectroscopy coupled with computation to discern molecular structure. In this work they examine the low-energy tautomers of guanine.1 The four lowest energy guanine tautomers are shown in Figure 1. (Unfortunately, Alonso does not include the optimized coordinates of these structures in the supporting information – we need to more vigorously police this during the review process!) These tautomers are predicted to be very close in energy (MP2/6-311++G(d,p), and so one might expect to see multiple signals in the microwave originating from all four tautomers. In fact, they discern all four, and the agreement between the computed and experimental rotational constants are excellent (Table 1), especially if one applies a scaling factor of 1.004. Once again, this group shows the power of combined experiment and computations!



1 (0.0) **2** (0.28)



3 (0.40) **4** (0.99)

Figure 1. Four lowest energy (kcal mol^{-1}, MP2/6-311++G(d,p)) tautomers of guanine.

Table 1. Experimental and computed rotational constants (MHz) of the four guanine tautomers.

	1		**2**		**3**		**4**	
	Exp	Comp	Exp	Comp	Exp	Comp	Exp	Comp
A	19.22155	1909.0	19.222780	1909.7	1916.080	1908.6	1923.460	1915.6
B	1121.6840	119.2	1116.6710	1113.5	1132.360	1128.2	1136.040	1131.9
C	709.0079	706.6	706.8580	704.2	712.1950	709.5	714.7000	712.0

Source: http://comporgchem.com/blog/?p=412