

Table 1. Rotational constants (MHz) for **1-5**.

	1		2		3		4		5	
	Expt	calc	Expt	calc	Expt	calc	Expt	calc	Expt	calc
<i>A</i>	3951.85	3934.5	3889.46	3876.5	3871.55	3856.0	3848.18	3820.1	3861.30	3844.2
<i>B</i>	2008.96	1999.1	2026.32	2014.7	2024.98	2012.3	2026.31	2019.0	2011.41	1999.7
<i>C</i>	1332.47	1326.8	1332.87	1326.9	1330.34	1323.3	1327.99	1324.0	1323.20	1318.4

The experimental and computed relative free energies are listed in Table 2. There is both not a complete match of the relative energetic ordering of the tautomers, nor is there good agreement in their magnitude. Previous computations² at CCSD(T)/cc-pVQZ//CCSD//cc-pVTZ are in somewhat better agreement with the gas-phase experiments.

Table 2. Relative free energies (kcal mol⁻¹) of **1-5**.

	expt	MP2/ 6-311++G(d,p)	CCSD(T)/cc-pVQZ// CCSD//cc-pVTZ
1	0.0	0.0	0.0
2	0.47	0.70	0.7
3	0.11	1.19	0.2
4	0.83	3.61	0.7
5		5.22	

Source: <http://comporgchem.com/blog/?p=2613>