

**Supplementary material:**

**Tables S3. Calculated and measured  $^1\text{H}$  (a) and  $^{13}\text{C}$  (b) chemical shifts for orotic acid;  $\text{H}_3\text{L}$ , and the hydroorotate anion,  $\text{H}_2\text{L}^-$ .**

**a) Calculated and measured  $^1\text{H}$  chemical shifts**

	Calculated				Experimental	
	Orotic acid B3LYP HF/6-311		Hydroorotate anion B3LYP HF/6-311		M $\text{H}_2\text{L}^{(a)}$	Ag $\text{H}_2\text{L}$
H1	7.244	7.188	6.524	6.481	10.57	10.59
H3	7.631	7.377	9.962	9.610	11.24	11.24
H5	6.408	6.250	6.050	5.781	6.18	6.20
Hc	6.509	6.718	-	-	-	-

(a) M =  $\text{NH}_4^+$ ,  $\text{Li}^+$ ,  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Cs}^+$ ,  $\text{Rb}^+$

**b) Calculated and measured  $^{13}\text{C}$  chemical shifts**

	Calculated				Experimental
	Orotic acid B3LYP HF/6-311		Hydroorotate anion B3LYP HF/6-311		Hydroorotate anion $^{(b)}$
C2	152.661	158.362	155.399	162.003	155.00
C4	167.066	172.257	171.600	178.195	170.29
C5	111.774	110.293	99.975	95.539	103.87
C6	143.856	147.375	161.392	169.166	150.97
C7	169.749	171.888	164.168	169.165	167.36

(b) G. Maistralis, A. Koutsodimou and N. Katsaros. *Trans. Met. Chem.* 2000, **25**, 166.

**Atomic numbering scheme:**

