

Supplementary material:

Tables S4. Observed and calculated IR frequencies for selected vibrations of orotic acid and the hydroorotate anion.

Orotic acid, H ₃ L						
Observed		Calculated (ref. 1)		Calculated (this work)		
v (cm ⁻¹)		v (cm ⁻¹)	assignment	v (cm ⁻¹)	I _{rel}	assignment
3241	sh	3796	v (O-H)	3696	0.17	v (O-H)
3154	m, broad	3637	v (N ₁ -H)	3603	0.07	v (N ₃ -H)
3137	m, broad	3614	v (N ₃ -H)	3601	0.27	v (N ₁ -H)
3099	sh	3266	v (C-H)	3285	0.01	v (C-H)
1729	vs	1858	v (O=O ₁)	1849	0.94	v (O=O ₃)
1719	vs	1849	v (C=O ₃)	1826	0.46	v (C=O ₁)
1700	vs	1807	v (C=O ₄)	1805	1.00	v (C=O ₄)
1653	vs	1698	v (C=C)	1688	0.07	v (C=C)

1) A. Hernanz, F. Billes, I. Bratu and R. Navarro. *Biopolymers*, 2000, 57, 187. (DFT - Becke3P86/6-311G**)

Hydroorotate anion, H ₂ L ⁻						
KH ₂ L (s), observed		Ag ₂ (H ₂ L) ₂ · 2 H ₂ O (s), observed		H ₂ L ⁻ , calculated		
v (cm ⁻¹)		v (cm ⁻¹)		v (cm ⁻¹)	I _{rel}	assignment
-	-	3450	broad	-	-	v _{s, as} (H ₂ O)
3158	m	3150	m	3620	0.06	v (N ₃ -H)
3108	m	3100	m	3453	0.51	v (N ₁ -H)
3087	m	3000	m	3268	0.002	v (C-H)
1705	sh	1700	sh	1807	1.00	v (O=O ₃)
1677	sh	1672	sh	1782	0.96	v _{asym} (COO)
1676	broad	1670	broad	1768	1.90	v (C=O ₄)
1615	m	1620	m	1664	0.17	v (C=C)
1492	m	1490	m	1495	0.52	Ring vibration
1472	w	1473	w	1405	0.03	Ring vibration
1423	w	1415	w	1385	0.02	δ (N-H)
1377	sh	1375	sh	1342	0.73	v _{sym} (COO)
1311	w	1305	m	1280	0.01	δ (N-H)