Supporting Information

Raman and computational study on the adsorption of xanthine on silver nanocolloids

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TABLE S1. Observed Raman frequencies of xanthine.

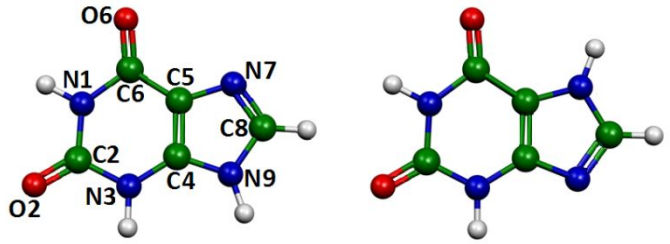
Raman solid (2004) [1]	Raman solid (2005) [2]	Raman solid (2011) [3]	Raman solid (2018) [4]	Raman pH=6 (2018) [4]	Raman pH=12 (2018) [4]	SERS Ag colloid [4]
482 (w)	487 (w)	464 (vw)	483 (w)	498 (w)	502 (w)	516
541 (s)	547 (ms)		542 (s)	562 (w/m)	566 (w)	575
616 (w)	622 (w)	602 (ms)	618 (vw)			
653 (vs)	658 (vs)	662 (vs)	653 (vs)	646(vs)	648 (vs)	657
838 (vw)	843 (w)	840 (vw)	839 (vw)	838 (vw)		
				870 (vw)		870
958 (s)	964 (s)	958 (s)	959 (s/m)	948 (m)	963 (w)	957
	1040 (w)	1025 (vw)	1034 (vw)	1038 (w)	1042 (vw)	
1127 (s)	1132 (w)		1129 (w)	1122 (w)	1136 (w)	1132
				1146 (w)		
				1190 (w/m)	1183 (m)	
1207 (s)	1212 (ms)	1208 (s)	1208 (m)	1208 (w)	1212 (m)	1223
1263 (s)	1268 (ms)		1264 (m)	1282 (s)	1273 (s)	1245
1339 (vs)	1335 (vs)	1315 (vs)	1329 (vs)	1318 (w)	1304 (w)	1320
					1352 (s)	1364
						1380
1422 (s)		1408 (s)	1434 (m/s)	1413 (w/m)	1422 (m)	1430
1490 (vw)			1490 (w)	1468 (s)		1476
1554 (s)	1560 (s)	1540 (s)	1555 (m/s)	1550 (sh)	1518 (s)	1551
1595 (w)	1600 (ms)	1572 (ms)	1596 (w)	1594 (w)	1586 (sh)	1573
1680 (w)	1685 (ms)	1689 (ms)	1680 (m)	1695 (sh)	1695 (sh)	1704

(1) Krishnakumar, M; Arivazhagan, M. *Indian J. Pure Appl. Phys.* **2004***, 24*, 411-418.
(2) Gunasekaran, S.; Sankari, G.; Ponnusamy, S. *Spectrochim. Acta A* **2005***, 61,* 117-127.
(3) Arivazhagan, M.; Jeyavijayan, S. *Spectrochim. Acta A* **2011***, 79,* 161-168.
(4) Present investigation.

TABLE S2. Calculated energies and molecule→metal electronic charge-transfers in silver complexes*.

	Calc. N(9)H-A complex	Calc. N(9)H-B Complex	Calc. N(7)H-A complex	Calc. N(7)H-B complex	Calc. N(7)H-C complex
Energy (Hartree)	-709.5009	-709.4645	-709.4818	-709.4811	-709.4819
molecule→metal charge-transfer	0.518 *e*	0.384 *e*	0.446 *e*	0.405 *e*	0.384 *e*

***** B3LYP/def2TZVPP basis set



N(9)H tautomer **N(7)H tautomer**

TABLE S3. Hirshfeld atomic charges*

Atom	N(9)H-A complex	N(9)H-B complex	N(7)H-A complex	N(7)H-B complex	N(7)H-C complex
N1	0.109361	0.070291	0.093752	0.075769	0.073635
C2	0.252625	0.245506	0.243480	0.245420	0.247433
N3	0.104202	0.107502	0.072765	0.124735	0.124172
C4	0.128783	0.107219	0.109661	0.121305	0.102321
C5	- 0.001282	0.010652	0.022615	0.005160	0.011411
C6	0.196533	0.199811	0.188484	0.185549	0.186732
N7	- 0.134096	-0.175460	0.177145	0.127286	0.141526
C8	0.218368	0.193247	0.217322	0.229252	0.216426
N9	0.142965	0.112908	- 0.123182	-0.198386	-0.206421
O2	- 0.266473	-0.237047	- 0.281653	-0.282827	-0.236879
O6	- 0.232830	-0.251116	- 0.274588	-0.228232	-0.276578
Ag	0.481949	0.616387	0.553847	0.595283	0.616151

* hydrogens summed into heavy atoms; B3LYP/def2TZVPP basis set.

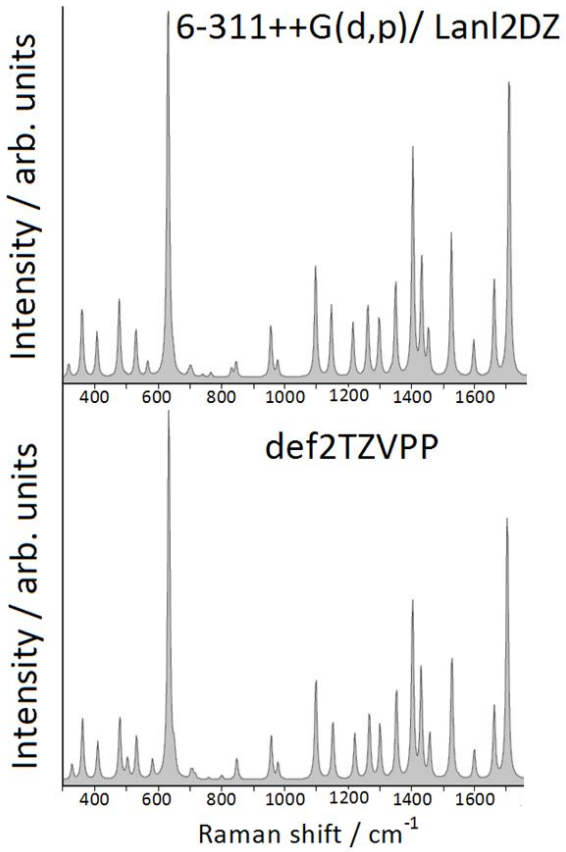


Figure S1. Comparison between the simulated SERS spectra of the N(9)H-A complex, obtained with the 6-311G++(d,p)/Lanl2DZ and def2TZVPP basis sets.