"Real Chemical States of the 3‑ Sulfur Derivative of 1,2,4-Triazole in Different Conditions: Complex Experimental and Theoretical Studies"

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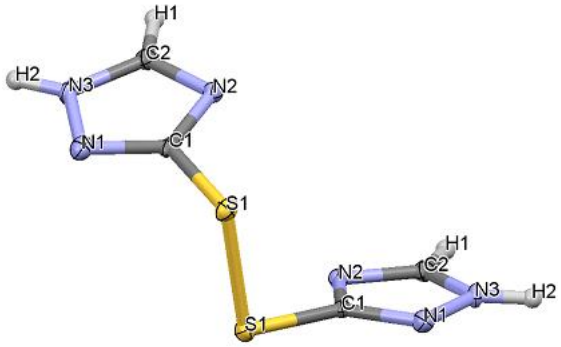

Figure S1. The molecular structure and atom labeling of 1,2-di(1H-1,2,4-triazol-3-yl)disulfane molecule.

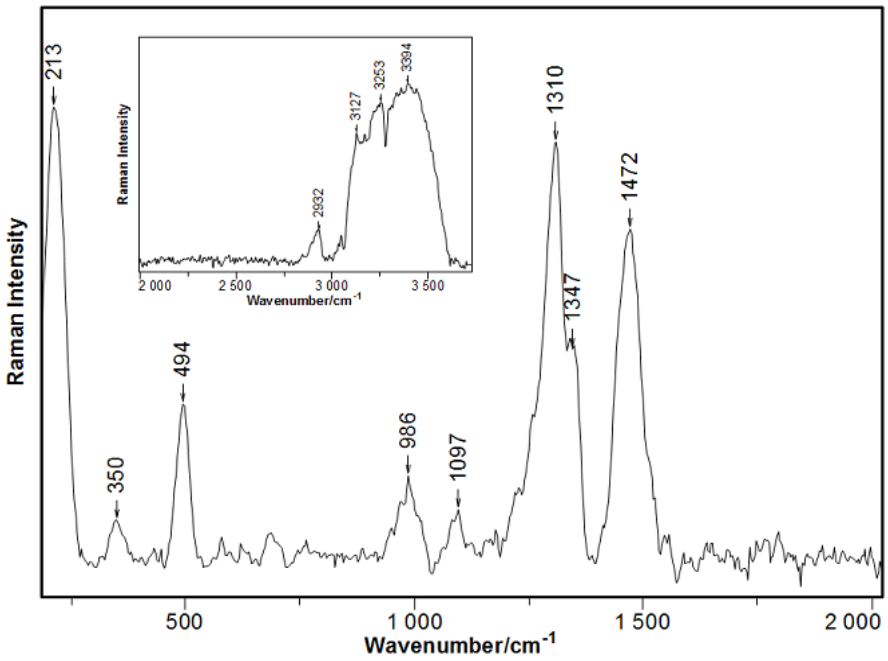

Figure S2. The SERS spectrum of TS adsorbed in 0.1 M solution of TS at pH 2.8 and transferred to 0.1 M solution of HCl; (λ_{ext}=514.5 nm).

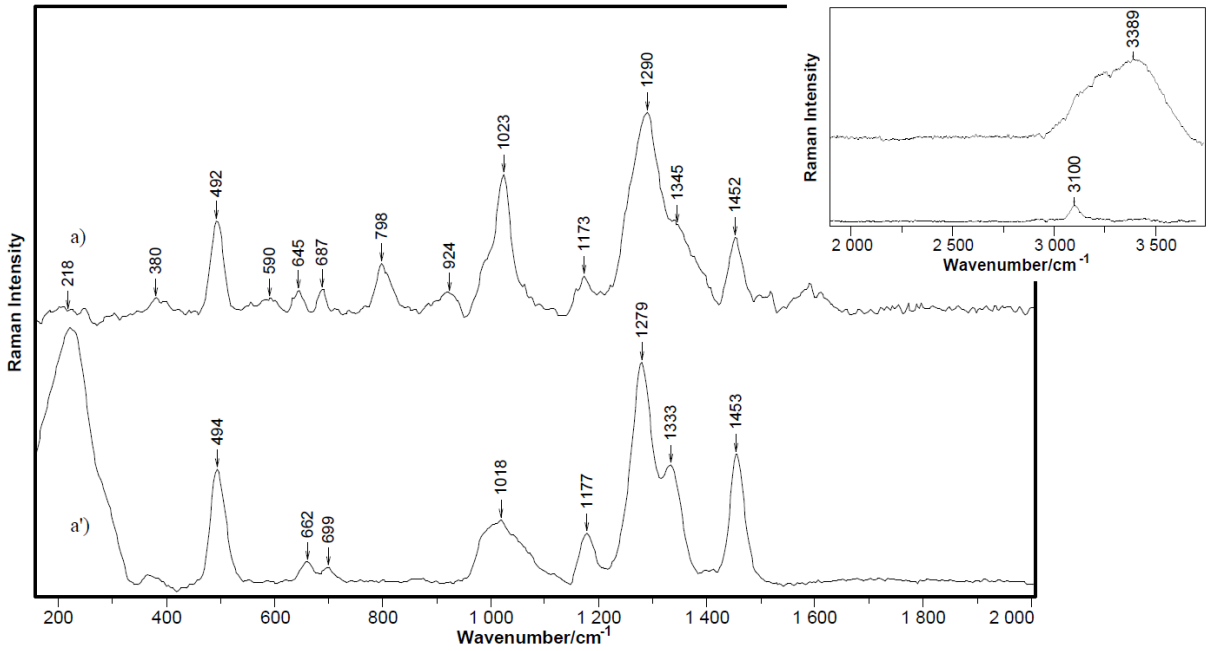

Figure S3. The Raman spectra of Ag-TS complexosalt (a) and the SERS spectra of TS monolayer adsorbed in 0.01 M TS solution at pH 12.3 (a') λ_{exc} = 514.5 nm. Bands around 800 and 1025 cm^{-1} are bands characteristic for a NO_3^- stretching mode.

Table S1. Selected bond lengths [Å] and angles [º] of 1,2-di(1H-1,2,4-triazol-3-yl)disulfane molecule.

bond	bond lengths [Å]	bond	bond angles [º]
S(1)-C(1)	1.7627(16)	C(1)-S(1)-S(1)	101.65(5)
S(1)-S(1)	2.0743(9)	N(1)-C(1)-N(2)	115.03(13)
C(1)-N(1)	1.3238(19)	N(1)-C(1)-S(1)	122.90(13)
C(1)-N(2)	1.361(2)	N(2)-C(1)-S(1)	122.07(11)
N(1)-N(3)	1.3573(19)	C(1)-N(1)-N(3)	101.76(13)
N(2)-C(2)	1.326(2)	C(2)-N(2)-C(1)	102.38(13)
N(3)-C(2)	1.329(2)	C(2)-N(3)-N(1)	110.55(13)
		N(2)-C(2)-N(3)	110.28(15)